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19. ABSTRACT (Continue on reverse if necessary and identify by block number)

An analysis of the reported spectra of five transition metal ions in yttrium aluminum garnet (YAG) is given. The reported data assumed that the ions occupied the $C_{3i}$ site in YAG, and this was also assumed in the analysis. The point charge lattice sums, $A_{nm}$, were calculated for the the $C_{3i}$ site, and the concept of rotational invariance was used to obtain a set of crystal field parameters, $B_{nm}$, for the triply ionized $3d^N$ electronic series. The energy levels for the entire ($Ti^{3+}$—$Zn^{3+}$) series of transition metal ions was calculated using the $B_{nm}$ for the $C_{3i}$ site. The spin-orbit interaction was included in the calculation.

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# Contents

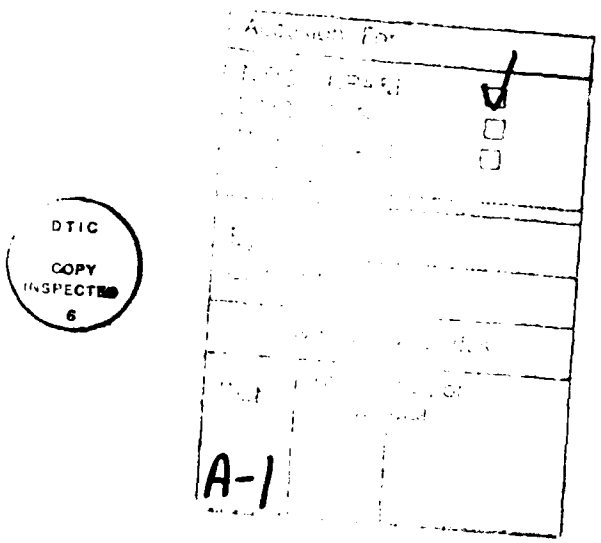


## Tables

**Tables** (cont'd)

# 1. Introduction

We report here on the analysis of the spectra of triply ionized transition metal ions, $X^{3+}$, with the electronic configuration $3d^N$ in the host lattice $Y_3Al_5O_{12}$ (YAG). The analysis is restricted predominantly to ions assumed to occupy the octahedral site ($C_{3i}$). Most of the experimental data on the $3d^N$ electronic configuration are for $N < 5$, with a large number of results for the $3d^3$ configuration, $Cr^{3+}$. The possibility that the $X^{3+}$ ions may occupy sites other than the $C_{3i}$ site (dodecahedral, $D_2$, or tetragonal, $S_4$) further complicates the analysis [1].* Further, much of the experimental data used in the analysis has been taken at room temperature, and any possibility of observing detailed electronic line structure is lost. Despite these shortcomings in the reported data, we analyze the existing data and formulate a method of calculating a set of parameters which can be used as first approximates to experimental energy levels. These parameters are used to calculate the energy levels of the entire $3d^N$ triply ionized transition elements. This latter calculation includes the full $C_{3i}$ symmetry as well as spin-orbit coupling.




*References are listed at the end of the text (p 36).

## 2. Free Ion and Crystal Field Interactions

The interaction considered in the analysis given here has been described in detail previously [2] and will be covered only briefly here. The free ion terms in the interaction contain the Slater parameters $F^{(2)}$ and $F^{(4)}$, and the configuration interaction contains the parameters $\alpha$ and $\gamma$. In the analysis here we shall assume $\gamma = 0$ throughout. The crystal field of $C_{3i}$ symmetry for the $nd^N$ configuration is

$$H_{CEF} = B_{20} \sum_{i=1}^{N} C_{20}(i) + B_{40} \sum_{i=1}^{N} C_{40}(i) + B_{43} \sum_{i=1}^{N} [C_{43}(i) - C_{4-3}(i)] ,$$
$$C_{nm}(i) = \sqrt{4\pi/(2n+1)}\ Y_{nm}(\theta_i, \Phi_i) , \tag{1}$$

where the crystal field parameter, $B_{43}$, is real and, for definiteness, with no loss in generality, we assume $B_{43}$ positive. For the cubic approximation in equation (1), we have

$$B_{20} = 0 ,$$
$$B_{43} = \sqrt{10/7}\ |B_{40}| . \tag{2}$$

(The $z$ axis of the crystal field is parallel to the $\langle 111 \rangle$ cubic axis.) The relationship of the crystal field parameters $B_{nm}$ to other notations is given by Konig and Kremer [3]. For ions in the $S_4$ site, the crystal field interaction is taken as

$$H_{CEF} = B_{20} \sum_{i=1}^{N} C_{20}(i) + B_{40} \sum_{i=1}^{N} C_{40}(i) + B_{44} \sum_{i=1}^{N} [C_{44}(i) + C_{4-4}(i)] , \tag{3}$$

where the crystal field parameter $B_{44}$ is real and assumed positive. In $S_4$ symmetry, the total crystal field interaction contains terms with $B_{32}$ and $B_{52}$. Both parameters are generally complex, but since we are considering interactions only in the $3d^N$ configuration, we shall ignore these terms. Further, it should be noted that since the odd terms $B_{32}$ and $B_{52}$ are present, electric dipole transitions can exist, and if they are present, their absorption intensity should be much larger [1] than for ions in the $C_{3i}$ site for which only magnetic dipole or electric quadrupole transitions are allowed. This, of course, has been recognized by others and has been used to identify the site occupancy of the ions, particularly $Fe^{3+}$ in YAG. The cubic approximation (tetrahedral) is obtained by letting

$$B_{20} = 0$$
$$B_{44} = \sqrt{5/14}\ |B_{40}| . \tag{4}$$

in equation (3) [3].

## 3. Analysis in the Cubic Approximation for the $C_{3i}$ Site

The reported parameters for the various ions $X^{3+}$ in YAG were used in a least-squares fit to the experimental data. Most of the data were analyzed in terms of $Dq$, $B$, and $C$. The relation of these parameters to our parameters is

$$F^{(2)} = 7(7B + C)$$
$$F^{(4)} = 63C/5$$
$$B_{40} = -14\,Dq\ ,$$

and $B_{43}$ given by equation (2). This latter relation is for $C_{3i}$ symmetry; however, for $S_4$ symmetry sites, $B_{40} = -21Dq$ and $B_{44}$ is given by equation (4). Starting with the parameters given in the references in table 1 [4–13] and the experimental data from these references, we obtained a best least-squares fit to the experimental data by varying $F^{(2)}$, $F^{(4)}$, $\alpha$, and $B_{40}$. These results are given in table 1. Tables 2 through 12 give the experimental and calculated energy levels from our fitting. In these tables $F^{(2)}$, $F^{(4)}$, $\alpha$, and $B_{40}$ were, in general, varied to obtain the best fit to the experimental data reported in the given references. For several ions the number of experimental energy levels did not exceed the number of parameters, and in these cases the results should be viewed accordingly. In particular the results obtained for $Co^{3+}$ are very questionable because of the large rms value with only six experimental energy levels.

**Table 1. Experimental values of $F^{(2)}$, $F^{(4)}$, $\alpha$, and $B_{40}$ for triply ionized transition metal ions, $X^{3+}$, in $Y_3Al_5O_{12}$**

| Ion | $nd^N$ | $F^{(2)}$ | $F^{(4)}$ | $\alpha$ | $B_{40}{}^{(a)}$ | Ref No. | Table No. |
|---|---|---|---|---|---|---|---|
| Ti | $3d^1$ | — | — | — | −25928 | 4 | 2 |
| V | $3d^2$ | 52164 | 38344 | 70 | −24104 | 5 | 3 |
| Cr | $3d^3$ | 60360 | 40020 | 0 | −22442 | 6 | 4 |
| Cr | $3d^3$ | 54870 | 36073 | 97 | −23116 | 7 | 5 |
| Cr | $3d^3$ | 56509 | 34680 | 110 | −22941 | 8 | 6 |
| Cr | $3d^3$ | 58125 | 44929 | 0 | −23978 | 9 | 7 |
| Cr | $3d^3$ | 54834 | 35666 | 122 | −22960 | 10 | 8 |
| Mn | $3d^4$ | 61762 | 41454 | 0 | −29419 | 11 | 9 |
| Fe | $3d^5$ | 49147 | 36324 | 23.8 | −17580 | 12 | 10 |
| Fe | $3d^5$ | 49280 | 37297 | 0 | −17703 | 13 | 11 |
| Co | $3d^6$ | 41033 | 22381 | 26.8 | −23292 | 11 | 12 |

[a] $B_{43} = \sqrt{10/7}\ |B_{40}|$

**Table 2. Energy levels ($cm^{-1}$) of $Ti^{3+}$ in $Y_3Al_5O_{12}$**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR[a] | Energy[b] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 1 | $^2T_2$ | 0 | −1 | 100 2D |
| 2 | $^2E$ | 18519 | 18519 | 100 2D |

*[a]In this and other tables which follow, IR is the irreducible representation of the cubic group.*
*[b]Experimental energy levels are taken from reference 4.*

**Table 3. Energy levels ($cm^{-1}$) of $V^{3+}$ in $Y_3Al_5O_{12}$**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 1 | $^3T_1$ | 0 | 0 | 91 3F + 9 3P |
| 2 | $^1T_2$ | 10256 | 10256 | 58 1D + 42 1G |
| 3 | $^1E$ | 0 | 10468 | 51 1D + 49 1G |
| 4 | $^3T_2$ | 16000 | 16000 | 100 3F |
| 5 | $^1A_1$ | 0 | 22142 | 68 1G + 32 1S |
| 6 | $^3T_1$ | 23530 | 23530 | 91 3P + 9 3F |
| 7 | $^1T_2$ | 0 | 27546 | 58 1G + 42 1D |
| 8 | $^1T_1$ | 0 | 30204 | 100 1G |
| 9 | $^3A_2$ | 0 | 33217 | 100 3F |
| 10 | $^1E$ | 0 | 44552 | 51 1G + 49 1D |
| 11 | $^1A_1$ | 0 | 58381 | 68 1S + 32 1G |

*[a]Experimental energy levels are taken from reference 5.*

**Table 4. Energy levels ($cm^{-1}$) of $Cr^{3+}$ in $Y_3Al_5O_{12}$**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 1 | $^4A_2$ | 0 | 124 | 100 4F |
| 2 | $^2E$ | 14500 | 15264 | 63 2G + 19 2H + 17 2D2 |
| 3 | $^2T_1$ | 0 | 15994 | 41 2G + 35 2H + 20 2P |
| 4 | $^4T_2$ | 16700 | 16154 | 100 4F |
| 5 | $^2T_2$ | 0 | 22621 | 35 2H + 27 2D1 + 1 2D2 |
| 6 | $^4T_1$ | 23200 | 23511 | 58 4F + 42 4P |
| 7 | $^2A_1$ | 0 | 28795 | 100 2G |
| 8 | $^2T_2$ | 31200 | 31187 | 58 2G + 38 2H + 3 2D2 |
| 9 | $^2T_1$ | 31200 | 31725 | 54 2H + 25 2G + 21 2P |
| 10 | $^2E$ | 0 | 33498 | 49 2H + 40 2D2 + 10 2D1 |
| 11 | $^4T_1$ | 36300 | 36498 | 58 4P + 42 4F |
| 12 | $^2T_1$ | 37800 | 36921 | 37 2H + 35 2P + 25 2F |
| 13 | $^2T_2$ | 43100 | 42673 | 56 2F + 41 2D2 + 2 2G |
| 14 | $^2A_2$ | 0 | 44357 | 100 2F |
| 15 | $^2T_1$ | 0 | 47324 | 68 2H + 32 2G |
| 16 | $^2T_2$ | 0 | 49268 | 26 2G + 25 2F + 22 2H |
| 17 | $^2E$ | 0 | 52404 | 43 2D2 + 24 2G + 17 2D1 |
| 18 | $^2T_1$ | 55000 | 55274 | 71 2F + 23 2P + 5 2H |
| 19 | $^2T_2$ | 0 | 71313 | 61 2D1 + 22 2D2 + 13 2F |
| 20 | $^2E$ | 0 | 71538 | 71 2D1 + 16 2H + 13 2G |

[a] *Experimental energy levels are taken from reference 6.*

**Table 5. Energy levels ($cm^{-1}$) of $Cr^{3+}$ in $Y_3Al_5O_{12}$**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 1 | $^4A_2$ | 0 | 138 | 100 4F |
| 2 | $^2E$ | 14559 | 14592 | 62 2G + 20 2D2 + 17 2H |
| 3 | $^2T_1$ | 15265 | 15247 | 38 2G + 33 2H + 24 2P |
| 4 | $^4T_2$ | 16700 | 16650 | 100 4F |
| 5 | $^2T_2$ | 21281 | 21278 | 30 2H + 30 2D1 + 20 2D2 |
| 6 | $^4T_1$ | 23200 | 23146 | 51 4P + 49 4F |
| 7 | $^2A_1$ | 0 | 28858 | 100 2G |
| 8 | $^2T_2$ | 0 | 31407 | 57 2G + 40 2H + 3 2D2 |
| 9 | $^2T_1$ | 0 | 31551 | 39 2H + 30 2G + 29 2P |
| 10 | $^2E$ | 0 | 32924 | 49 2H + 41 2D2 + 10 2D1 |
| 11 | $^2T_1$ | 0 | 36171 | 52 2H + 25 2F + 22 2P |
| 12 | $^4T_1$ | 36300 | 36357 | 51 4F + 49 4P |
| 13 | $^2T_2$ | 0 | 40606 | 60 2F + 38 2D2 + 2 2G |
| 14 | $^2A_2$ | 0 | 42298 | 100 2F |
| 15 | $^2T_1$ | 0 | 48295 | 69 2H + 31 2G |
| 16 | $^2T_2$ | 0 | 48888 | 29 2G + 25 2H + 19 2F |
| 17 | $^2E$ | 0 | 50425 | 39 2D2 + 27 2D1 + 21 2G |
| 18 | $^2T_1$ | 0 | 53834 | 69 2F + 24 2P + 7 2H |
| 19 | $^2T_2$ | 0 | 68067 | 59 2D1 + 22 2D2 + 15 2F |
| 20 | $^2E$ | 0 | 70007 | 61 2D1 + 21 2H + 17 2G |

[a] *Experimental energy levels are taken from reference 7.*

**Table 6. Energy levels ($cm^{-1}$) of $Cr^{3+}$ in $Y_3Al_5O_{12}$**

*[Theoretical levels were calculated with parameters in table 1]*

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 1 | $^4A_2$ | 0 | 16 | 100 4F |
| 2 | $^2E$ | 14616 | 14523 | 62 2G + 20 2D2 + 16 2H |
| 3 | $^2T_1$ | 15200 | 15255 | 39 2G + 32 2H + 25 2P |
| 4 | $^4T_2$ | 16400 | 16402 | 100 4F |
| 5 | $^2R_2$ | 21100 | 21110 | 31 2D1 + 29 2H + 21 2D2 |
| 6 | $^4T_1$ | 23200 | 23187 | 52 4F + 48 4P |
| 7 | $^2A_1$ | 0 | 28579 | 100 2G |
| 8 | $^2T_2$ | 0 | 31307 | 57 2G + 40 2H + 3 2D2 |
| 9 | $^2T_1$ | 0 | 31432 | 37 2H + 31 2P + 30 2G |
| 10 | $^2E$ | 0 | 32783 | 49 2H + 40 2D2 + 11 2D1 |
| 11 | $^2T_1$ | 0 | 36300 | 54 2H + 24 2F + 22 2P |
| 12 | $^4T_1$ | 36300 | 36304 | 52 4P + 48 4F |
| 13 | $^2T_2$ | 0 | 41060 | 58 2F + 39 2D2 + 2 2G |
| 14 | $^2A_2$ | 0 | 42900 | 100 2F |
| 15 | $^2T_1$ | 0 | 48153 | 70 2H + 30 2G |
| 16 | $^2T_2$ | 0 | 48699 | 27 2G + 26 2H + 21 2F |
| 17 | $^2E$ | 0 | 50858 | 40 2D2 + 25 2D1 + 21 2G |
| 18 | $^2T_1$ | 0 | 54084 | 70 2F + 23 2P + 7 2H |
| 19 | $^2T_2$ | 0 | 68579 | 58 2D1 + 23 2D2 + 15 2F |
| 20 | $^2E$ | 0 | 69692 | 62 2D1 + 21 2H + 16 2G |

[a] *Experimental energy levels are taken from reference 8.*

**Table 7. Energy levels ($cm^{-1}$) of $Cr^{3+}$ in $Y_3Al_5O_{12}$**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 1 | $^4A_2$ | 0 | −132 | 100 4F |
| 2 | $^2E$ | 0 | 15593 | 61 2G + 19 2H + 18 2D2 |
| 3 | $^2T_1$ | 0 | 16164 | 39 2G + 35 2H + 21 2P |
| 4 | $^4T_2$ | 16950 | 16995 | 100 4F |
| 5 | $^2T_2$ | 0 | 23329 | 38 2H + 27 2D1 + 17 2D2 |
| 6 | $^4T_1$ | 23730 | 23783 | 50 4P + 50 4F |
| 7 | $^2A_1$ | 0 | 30400 | 100 2G |
| 8 | $^2T_2$ | 0 | 32556 | 58 2G + 37 2H + 4 2D2 |
| 9 | $^2T_1$ | 0 | 32946 | 55 2H + 25 2G + 20 2P |
| 10 | $^2E$ | 0 | 34794 | 49 2H + 43 2D2 + 9 2D1 |
| 11 | $^4T_1$ | 37540 | 37486 | 50 4F + 50 4P |
| 12 | $^2T_1$ | 0 | 37700 | 36 2H + 32 2P + 29 2F |
| 13 | $^2T_2$ | 0 | 42524 | 62 2F + 37 2D2 + 1 2G |
| 14 | $^2A_2$ | 0 | 43936 | 100 2F |
| 15 | $^2T_1$ | 0 | 49675 | 67 2H + 33 2G |
| 16 | $^2T_2$ | 0 | 51438 | 29 2G + 22 2D2 + 21 2H |
| 17 | $^2E$ | 0 | 52976 | 39 2D2 + 24 2D1 + 23 2G |
| 18 | $^2T_1$ | 0 | 56329 | 66 2F + 27 2P + 7 2H |
| 19 | $^2T_2$ | 0 | 72119 | 63 2D1 + 19 2D2 + 14 2F |
| 20 | $^2E$ | 0 | 74668 | 66 2D1 + 18 2H + 15 2G |

[a]*Experimental energy levels are taken from reference 9.*

**Table 8. Energy levels ($cm^{-1}$) of $Cr^{3+}$ in $Y_3Al_5O_{12}$**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 1 | $^4A_2$ | 0 | 1 | 100 4F |
| 2 | $^2E$ | 14542 | 14541 | 61 2G + 21 2D2 + 16 2H |
| 3 | $^2T_1$ | 15200 | 15199 | 38 2G + 32 2H + 25 2P |
| 4 | $^4T_2$ | 16400 | 16401 | 100 4F |
| 5 | $^2T_2$ | 21100 | 21100 | 31 2D1 + 29 2H + 21 2D2 |
| 6 | $^4T_1$ | 0 | 22789 | 51 4P + 49 4F |
| 7 | $^2A_1$ | 0 | 28727 | 100 2G |
| 8 | $^2T_2$ | 0 | 31373 | 56 2G + 40 2H + 3 2D2 |
| 9 | $^2T_1$ | 0 | 31385 | 35 2H + 32 2P + 31 2G |
| 10 | $^2E$ | 0 | 32741 | 49 2H + 41 2D2 + 10 2D1 |
| 11 | $^2T_1$ | 0 | 35913 | 51 4F + 49 4P |
| 12 | $^4T_1$ | 0 | 36059 | 56 2H + 24 2F + 19 2P |
| 13 | $^2T_2$ | 0 | 40290 | 60 2F + 38 2D2 + 2 2G |
| 14 | $^2A_2$ | 0 | 42045 | 100 2F |
| 15 | $^2T_1$ | 0 | 48240 | 69 2H + 30 2G |
| 16 | $^2T_2$ | 0 | 48595 | 29 2G + 26 2H + 19 2F |
| 17 | $^2E$ | 0 | 50105 | 38 2D2 + 28 2D1 + 21 2G |
| 18 | $^2T_1$ | 0 | 53436 | 69 2F + 23 2P + 8 2H |
| 19 | $^2T_2$ | 0 | 67566 | 58 2D1 + 22 2D2 + 15 2F |
| 20 | $^2E$ | 0 | 69492 | 60 2D1 + 22 2H + 17 2G |

[a]*Experimental energy levels are taken from reference 10.*

**Table 9. Energy levels ($cm^{-1}$) of $Mn^{3+}$ in $Y_3Al_5O_{12}$**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 1 | $^3T_1$ | 0 | 0 | 40 3H + 17 3G + 16 3F1 |
| 2 | $^5E$ | 0 | 1087 | 100 5D |
| 3 | $^1T_2$ | 0 | 9356 | 35 1I + 28 1G2 + 23 1G1 |
| 4 | $^1E$ | 0 | 10500 | 57 1I + 22 1D2 + 11 1G1 |
| 5 | $^3E$ | 0 | 18226 | 84 3H + 15 3G + 1 3D |
| 6 | $^1A_1$ | 0 | 18869 | 38 1G1 + 24 1I + 20 1S2 |
| 7 | $^3T_1$ | 0 | 19072 | 45 3H + 23 3G + 19 3P2 |
| 8 | $^3T_2$ | 0 | 19913 | 41 3F2 + 32 3H + 13 3F1 |
| 9 | $^3A_1$ | 0 | 21361 | 100 3G |
| 10 | $^5T_2$ | 22100 | 22100 | 100 5D |
| 11 | $^1T_2$ | 0 | 22154 | 94 3F2 + 6 3F1 |
| 12 | $^3E$ | 0 | 24733 | 56 3D + 41 3G + 3 3H |
| 13 | $^1A_2$ | 0 | 27162 | 91 1I + 9 1F |
| 14 | $^1T_2$ | 27200 | 27200 | 61 1I + 23 1G2 + 7 1G1 |
| 15 | $^1T_1$ | 0 | 29443 | 40 1I + 24 1G2 + 20 1G1 |
| 16 | $^1E$ | 31500 | 31500 | 41 1D2 + 33 1G2 + 20 1I |
| 17 | $^3T_1$ | 0 | 32447 | 35 3G + 27 3H + 25 3P1 |
| 18 | $^3T_2$ | 0 | 34073 | 39 3D + 32 3F1 + 23 3G |
| 19 | $^3T_1$ | 0 | 39507 | 52 3H + 32 3F2 + 6 3F1 |
| 20 | $^3T_2$ | 0 | 40957 | 56 3H + 21 3F2 + 11 3D |
| 21 | $^1A_1$ | 0 | 41615 | 62 1G2 + 18 1S2 + 16 1G1 |
| 22 | $^1T_1$ | 0 | 43564 | 37 1F + 24 1G1 + 22 1G2 |
| 23 | $^3T_2$ | 0 | 43717 | 44 3G + 43 3D + 12 3H |
| 24 | $^1T_2$ | 0 | 44831 | 62 1F + 19 1D1 + 13 1G1 |
| 25 | $^3T_2$ | 0 | 45135 | 40 3G + 33 3F2 + 24 3D |
| 26 | $^1T_2$ | 0 | 47185 | 85 1I + 9 1G2 + 3 1G1 |
| 27 | $^3T_1$ | 0 | 48161 | 57 3P2 + 20 3G + 17 3F2 |
| 28 | $^1E$ | 0 | 48262 | 43 1G2 + 26 1G1 + 22 1I |
| 29 | $^1A_1$ | 0 | 49786 | 41 1I + 29 1S2 + 18 1G2 |
| 30 | $^1T_2$ | 0 | 56126 | 70 1D2 + 11 1I + 9 1G1 |
| 31 | $^1A_2$ | 0 | 56846 | 91 1F + 9 1I |
| 32 | $^1T_1$ | 0 | 57683 | 53 1G2 + 46 1F + 1 1I |
| 33 | $^3T_1$ | 0 | 59751 | 71 3F1 + 19 3H + 6 3P2 |

**Table 9. Energy levels ($cm^{-1}$) of $Mn^{3+}$ in $Y_3Al_5O_{12}$ (cont'd)**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 34 | $^3A_2$ | 0 | 62517 | 94 3F1 + 6 3F2 |
| 35 | $^1E$ | 0 | 67079 | 62 1G1 + 23 1G2 + 11 1D2 |
| 36 | $^3T_1$ | 0 | 68610 | 51 3P1 + 27 3F2 + 13 3H |
| 37 | $^1T_1$ | 0 | 72164 | 55 1G1 + 43 1I + 1 1F |
| 38 | $^3T_2$ | 0 | 73296 | 53 3F1 + 19 3G + 19 3D |
| 39 | $^1T_2$ | 0 | 76810 | 28 1G1 + 28 1D1 + 22 1D2 |
| 40 | $^1A_1$ | 0 | 84593 | 27 1S2 + 26 1I + 23 1G1 |
| 41 | $^1E$ | 0 | 86023 | 79 1D1 + 20 1D2 + 1 1I |
| 42 | $^1T_2$ | 0 | 86877 | 41 1D1 + 23 1F + 17 1G2 |
| 43 | $^1A_1$ | 0 | 108559 | 66 1S1 + 23 1G1 + 6 1S2 |

[a]*Experimental energy levels are taken from reference 11.*

**Table 10. Energy levels ($cm^{-1}$) of $Fe^{3+}$ in $Y_3Al_5O_{12}$**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 1 | $^6A_1$ | 0 | −2 | 100 6S |
| 2 | $^4T_1$ | 10400 | 10400 | 59 4G + 38 4P + 3 4F |
| 3 | $^2T_2$ | 0 | 10827 | 30 2I + 26 2H + 19 2F1 |
| 4 | $^4T_2$ | 14300 | 14309 | 46 4G + 29 4F + 25 4D |
| 5 | $^2A_2$ | 0 | 20610 | 54 2I + 42 2F1 + 4 2F2 |
| 6 | $^4(A_1,E)$ | 20717 | 20800 | 100 4G |
| 7 | $^2T_1$ | 0 | 20931 | 58 2I + 24 2H + 14 2F1 |
| 8 | $^2T_2$ | 0 | 22075 | 48 2I + 24 2F1 + 12 2H |
| 9 | $^4T_2$ | 22880 | 22679 | 55 4D + 43 4G + 2 4F |
| 10 | $^2E$ | 0 | 23473 | 33 2I + 31 2H + 15 2D3 |
| 11 | $^4E$ | 24440 | 24605 | 100 4D |
| 12 | $^2T_1$ | 0 | 26897 | 32 2G2 + 21 2F1 + 20 2H |
| 13 | $^2T_2$ | 0 | 28889 | 30 2G2 + 25 2F2 + 14 2I |
| 14 | $^2A_1$ | 0 | 29251 | 62 2I + 19 2G2 + 13 2G1 |
| 15 | $^4T_1$ | 0 | 30530 | 46 4F + 42 4P + 13 4G |

**Table 10. Energy levels ($cm^{-1}$) of $Fe^{3+}$ in $Y_3Al_5O_{12}$ (cont'd)**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 16 | $^2E$ | 0 | 30665 | 47 2I + 26 2D3 + 13 2D1 |
| 17 | $^2T_2$ | 0 | 32011 | 51 2I + 36 2D3 + 8 2D1 |
| 18 | $^2A_1$ | 0 | 32131 | 44 2G2 + 37 2I + 11 2G1 |
| 19 | $^4A_2$ | 0 | 33470 | 100 4F |
| 20 | $^2E$ | 0 | 34902 | 74 2G2 + 11 2I + 5 2D3 |
| 21 | $^2T_2$ | 0 | 36135 | 45 2F2 + 26 2G2 + 16 2I |
| 22 | $^2T_1$ | 0 | 36592 | 68 2H + 30 2F1 + 1 2G2 |
| 23 | $^2A_2$ | 0 | 36949 | 71 2F2 + 22 2I + 7 2F1 |
| 24 | $^2T_1$ | 0 | 37093 | 48 2F2 + 39 2G2 + 9 2I |
| 25 | $^4T_1$ | 0 | 37704 | 51 4F + 29 4G + 20 4P |
| 26 | $^2A_1$ | 0 | 39945 | 69 2S + 27 2G2 + 4 2G1 |
| 27 | $^2E$ | 0 | 40975 | 41 2H + 33 2D3 + 25 2D2 |
| 28 | $^4T_2$ | 0 | 41888 | 69 4F + 21 4D + 10 4G |
| 29 | $^2T_1$ | 0 | 42283 | 37 2H + 19 2F2 + 18 2F1 |
| 30 | $^2T_2$ | 0 | 43413 | 31 2F1 + 19 2H + 15 2G2 |
| 31 | $^2T_1$ | 0 | 46706 | 43 2H + 30 2I + 16 2F1 |
| 32 | $^2A_2$ | 0 | 46747 | 51 2F1 + 25 2F2 + 24 2I |
| 33 | $^2E$ | 0 | 49269 | 72 2G1 + 9 2H + 8 2D1 |
| 34 | $^2T_2$ | 0 | 51523 | 53 2D2 + 13 2G1 + 12 2I |
| 35 | $^2E$ | 0 | 52402 | 54 2D2 + 11 2G1 + 11 2G2 |
| 36 | $^2T_2$ | 0 | 53835 | 25 2D3 + 25 2H + 16 2I |
| 37 | $^2T_1$ | 0 | 54302 | 78 2G1 + 8 2P + 6 2F2 |
| 38 | $^2T_2$ | 0 | 57447 | 47 2G1 + 13 2G2 + 12 2F2 |
| 39 | $^2A_1$ | 0 | 59526 | 72 2G1 + 17 2S + 11 2G2 |
| 40 | $^2T_1$ | 0 | 63651 | 86 2P + 5 2F2 + 5 2G2 |
| 41 | $^2T_2$ | 0 | 73086 | 66 2D1 + 7 2H + 7 2D3 |
| 42 | $^2E$ | 0 | 73251 | 67 2D1 + 13 2D3 + 12 2G1 |

[a] *Experimental energy levels are taken from reference 12.*

**Table 11. Energy levels ($cm^{-1}$) of $Fe^{3+}$ in $Y_3Al_5O_{12}$**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 1 | $^6A_1$ | 0 | −1 | 100 6S |
| 2 | $^4T_1$ | 10360 | 10377 | 60 4G + 37 4P + 4 4F |
| 3 | $^2T_2$ | 0 | 10680 | 32 2I + 27 2H + 18 2F1 |
| 4 | $^4T_2$ | 14200 | 14195 | 48 4G + 29 4F + 24 4D |
| 5 | $^2A_2$ | 0 | 20438 | 56 2I + 41 2F1 + 4 2F2 |
| 6 | $^2T_1$ | 0 | 20610 | 60 2I + 24 2H + 13 2F1 |
| 7 | $^4(A_1,E)$ | 20530 | 20627 | 100 4G |
| 8 | $^2T_2$ | 0 | 21874 | 49 2I + 24 2F1 + 11 2H |
| 9 | $^4T_2$ | 22940 | 22659 | 55 4D + 42 4G + 3 4F |
| 10 | $^2E$ | 0 | 23329 | 36 2I + 30 2H + 14 2D3 |
| 11 | $^4E$ | 24450 | 24707 | 100 4D |
| 12 | $^2T_1$ | 0 | 26902 | 33 2G2 + 21 2F1 + 20 2H |
| 13 | $^2T_2$ | 0 | 28814 | 30 2G2 + 24 2F2 + 17 2I |
| 14 | $^2A_1$ | 0 | 28912 | 68 2I + 16 2G2 + 11 2G1 |
| 15 | $^2E$ | 0 | 30639 | 47 2I + 25 2D3 + 13 2D1 |
| 16 | $^4T_1$ | 0 | 30741 | 47 4F + 42 4P + 11 4G |
| 17 | $^2T_1$ | 0 | 31947 | 48 2G2 + 31 2I + 13 2G1 |
| 18 | $^2T_2$ | 0 | 31985 | 48 2I + 37 2D3 + 8 2D1 |
| 19 | $^4A_2$ | 0 | 33542 | 100 4F |
| 20 | $^2E$ | 0 | 34885 | 74 2G2 + 9 2I + 6 2D3 |
| 21 | $^2T_2$ | 0 | 36158 | 45 2F2 + 25 2G2 + 15 2I |
| 22 | $^2T_1$ | 0 | 36678 | 69 2H + 30 2F1 + 1 2G2 |
| 23 | $^2A_2$ | 0 | 36961 | 71 2F2 + 21 2I + 8 2F1 |
| 24 | $^2T_1$ | 0 | 37090 | 48 2F2 + 39 2G2 + 9 2I |
| 25 | $^4T_1$ | 0 | 37850 | 50 4F + 29 4G + 22 4P |
| 26 | $^2A_1$ | 0 | 40168 | 69 2S + 26 2G2 + 4 2G1 |
| 27 | $^2E$ | 0 | 41121 | 40 2H + 35 2D3 + 25 2D2 |
| 28 | $^4T_2$ | 0 | 42022 | 69 4F + 21 4D + 10 4G |
| 29 | $^2T_1$ | 0 | 42379 | 36 2H + 20 2F2 + 18 2F1 |
| 30 | $^2T_2$ | 0 | 43560 | 31 2F1 + 20 2H + 15 2G2 |
| 31 | $^2T_1$ | 0 | 46693 | 42 2H + 29 2I + 17 2F1 |
| 32 | $^2A_2$ | 0 | 46953 | 52 2F1 + 25 2F2 + 23 2I |
| 33 | $^2E$ | 0 | 49272 | 73 2G1 + 9 2H + 8 2D1 |

**Table 11. Energy levels ($cm^{-1}$) of $Fe^{3+}$ in $Y_3Al_5O_{12}$ (cont'd)**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 34 | $^2T_2$ | 0 | 51725 | 50 2D2 + 16 2G1 + 13 2I |
| 35 | $^2E$ | 0 | 52668 | 56 2D2 + 11 2G2 + 10 2H |
| 36 | $^2T_2$ | 0 | 54029 | 26 2D3 + 23 2H + 16 2F1 |
| 37 | $^2T_1$ | 0 | 54335 | 78 2G1 + 8 2P + 7 2F2 |
| 38 | $^2T_2$ | 0 | 57575 | 47 2G1 + 13 2G2 + 12 2F2 |
| 39 | $^2A_1$ | 0 | 59643 | 71 2G1 + 17 2S + 10 2G2 |
| 40 | $^2T_1$ | 0 | 63922 | 86 2P + 5 2F2 + 5 2G2 |
| 41 | $^2T_2$ | 0 | 73556 | 67 2D1 + 7 2H + 7 2D3 |
| 42 | $^2E$ | 0 | 73691 | 68 2D1 + 13 2D3 + 12 2G1 |

[a]*Experimental energy levels are taken from reference 13.*

**Table 12. Energy levels ($cm^{-1}$) of $Co^{3+}$ in $Y_3Al_5O_{12}$**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 1 | $^1A_1$ | 0 | −232 | 35 1G1 + 33 1I + 20 1G2 |
| 2 | $^3T_1$ | 0 | 11110 | 41 3H + 25 3F2 + 20 3P1 |
| 3 | $^3T_2$ | 14900 | 14919 | 38 3G + 24 3H + 23 3F1 |
| 4 | $^1T_1$ | 15600 | 15464 | 55 1I + 28 1G1 + 18 1G2 |
| 5 | $^5T_2$ | 0 | 16390 | 100 5D |
| 6 | $^1T_2$ | 22400 | 22672 | 27 1I + 21 1D2 + 20 1F |
| 7 | $^3T_1$ | 26600 | 26802 | 64 3H + 26 3F2 + 7 3F1 |
| 8 | $^3T_2$ | 0 | 27829 | 53 3H + 42 3G + 5 3F2 |
| 9 | $^3E$ | 29700 | 29359 | 52 3G + 29 3H + 19 3D |
| 10 | $^3T_1$ | 0 | 29359 | 48 3G + 32 3P2 + 11 3H |
| 11 | $^1E$ | 0 | 31597 | 45 1G2 + 30 1G1 + 22 1I |
| 12 | $^3T_2$ | 0 | 31673 | 54 3D + 43 3F2 + 4 3G |
| 13 | $^1T_2$ | 0 | 32124 | 69 1I + 12 1G2 + 10 1D2 |
| 14 | $^1A_1$ | 0 | 32352 | 52 1I + 28 1S2 + 10 1S1 |
| 15 | $^5E$ | 0 | 33027 | 100 5D |
| 16 | $^3A_2$ | 0 | 35959 | 74 3F1 + 26 3F2 |

**Table 12. Energy levels ($cm^{-1}$) of $Co^{3+}$ in $Y_3Al_5O_{12}$ (cont'd)**

***[Theoretical levels were calculated with parameters in table 1]***

| Level No. | IR | Energy[a] (exp) | Energy (theor) | Free-ion state (%) |
|---|---|---|---|---|
| 17 | $^1T_1$ | 0 | 36366 | 39 1G2 + 32 1F + 25 1I |
| 18 | $^1A_2$ | 0 | 37076 | 58 1F + 42 1I |
| 19 | $^1T_2$ | 0 | 37610 | 27 1D2 + 27 1F + 23 1I |
| 20 | $^3T_1$ | 0 | 40727 | 32 3H + 29 3F2 + 17 3F1 |
| 21 | $^1E$ | 0 | 41617 | 38 1D2 + 36 1G1 + 19 1D1 |
| 22 | $^3E$ | 0 | 43870 | 69 3H + 29 3G + 2 3D |
| 23 | $^3T_1$ | 0 | 44577 | 33 3G + 29 3P2 + 22 3H |
| 24 | $^3T_2$ | 0 | 44791 | 31 3F2 + 23 3H + 19 3D |
| 25 | $^1T_2$ | 0 | 44988 | 43 1G1 + 30 1I + 15 1D2 |
| 26 | $^3A_1$ | 0 | 45760 | 100 3G |
| 27 | $^3E$ | 0 | 48475 | 79 3D + 19 3G + 2 3H |
| 28 | $^1E$ | 0 | 48642 | 48 1I + 37 1G2 + 9 1D1 |
| 29 | $^1A_1$ | 0 | 50412 | 57 1G2 + 21 1S2 + 18 1S1 |
| 30 | $^1A_2$ | 0 | 50540 | 58 1I + 42 1F |
| 31 | $^1T_2$ | 0 | 51406 | 43 1G2 + 22 1I + 18 1F |
| 32 | $^1T_2$ | 0 | 51995 | 74 3F2 + 26 3F1 |
| 33 | $^1T_1$ | 0 | 52204 | 61 1F + 17 1I + 15 1G1 |
| 34 | $^3T_1$ | 0 | 57039 | 57 3P1 + 19 3F2 + 12 3P2 |
| 35 | $^3T_2$ | 0 | 57173 | 61 3F1 + 18 3F2 + 15 3D |
| 36 | $^1T_2$ | 0 | 60211 | 40 1G1 + 25 1I + 15 1D2 |
| 37 | $^1A_1$ | 0 | 60860 | 37 1S2 + 37 1G1 + 10 1S1 |
| 38 | $^1E$ | 0 | 61751 | 54 1D1 + 34 1D2 + 7 1G2 |
| 39 | $^1T_1$ | 0 | 62434 | 54 1G1 + 36 1G2 + 7 1F |
| 40 | $^3T_1$ | 0 | 64466 | 53 3F1 + 19 3H + 18 3G |
| 41 | $^1E$ | 0 | 71113 | 30 1G1 + 23 1D2 + 20 1I |
| 42 | $^1T_2$ | 0 | 76690 | 59 1D1 + 19 1F + 10 1D2 |
| 43 | $^1A_1$ | 0 | 87780 | 57 1S1 + 26 1G1 + 8 1S2 |

[a] *Experimental energy levels are taken from reference 11.*

# 4. Theoretical Crystal Field Parameters

## *4.1 Point Charge Crystal Field*

The crystallographic data of Euler and Bruce [14] on YAG are given in table 13. The yttrium site (24*c*) and the $Al_2$ site (24*d*) have been chosen to have the principal axis of each site along the crystallographic *c*-axis. The crystal field components, $A_{nm}$, for the $Al_2$ site are given in table 14. The various contributions to the $A_{nm}$ are individually given, but most of our analysis will center about the point charge values of $A_{nm}$ (for the dipole contribution, the polarizabilities of Schmidt et al [15] are used). In tetrahedral coordination ($Al_2$), the lattice sum components should be such that $|A_{44}/A_{40}| = (5/14)^{1/2}$, which for the point charge given in table 14, $|A_{44}/A_{40}| = 0.3928$, which is considerably less than the true tetrahedral value. From these results one would expect that a tetrahedral approximation to the analysis of ions occupying the $Al_2$ site would be a rather poor one. The corresponding $A_{nm}$ for the $Al_1$ site (16*a*) are given in table 15. In this table the crystal field components were first computed in the crystallographic coordinates and then rotated so that the principal axis of $C_{3i}$ was parallel to the (111) crystallographic axis. If the site were pure octahedral, we would have $|A_{43}/A_{40}| = (10/7)^{1/2} = 1.1952$, and for the point charge values of $A_{40}$ and $A_{43}$ of table 15, $|A_{43}/A_{40}| = 1.1243$, which is quite close to the octahedral value. Of course the $A_{20}$ value is significantly different from the octahedral value of zero.

In the point charge or point multipole theory of the crystal field interaction, the theoretical crystal field parameters are given by

$$B_{nm} = \rho_n A_{nm} \quad , \tag{6}$$

where the $A_{nm}$ are the crystal field components given in tables 14 and 15 and $\rho_n$ is an effective radial expectation value. To relate the theoretical $B_{nm}$ with those obtained by fitting the experimental data, we use the concept of a rotational invariant [16,17], which we define as

$$S_n(B) = \left( \sum_{m=-n}^{n} B_{nm}^{*} B_{nm} \right)^{1/2} \quad . \tag{7}$$

For $n = 4$ and $C_{3i}$ symmetry, we have

$$S_4(B) = \left(B_{40}^2 + 2B_{43}^2\right)^{1/2} \quad , \tag{8}$$

and from equation (6) we obtain

$$S_4(B) = \rho_4 \, S_4(A) \quad , \tag{9}$$

where

$$S_4(A) = \left(A_{40}^2 + 2A_{43}^2\right)^{1/2} \quad .$$

For cubic symmetry and using equation (2), we obtain

$$S_4(B) = \sqrt{27/7} \; |B_{40}^e| \quad , \tag{10}$$

where the $B_{40}^e$ are the experimental values given in table 1. The results of table 15 for the point charge $A_{4m}$ along with the $B_{40}^e$ given in table 1 were used to obtain $\rho_4$ with

$$\rho_4 = \frac{\sqrt{27/7} \; |B_{40}^e|}{S_4(A)} \quad . \tag{11}$$

In ions for which we have more than one set of data, we selectively average the $\rho_4$ obtained from equation (11). If we assume that the wavefunctions expand from the Hartree-Fock value, then we assume that

$$\rho_n = \langle r^n \rangle_{HF} \tau^n \quad , \tag{12}$$

where this result is obtained by assuming the radial wavefunction $R(r) = R_{HF}(\tau r)$. Using equation (12) we have

$$\frac{1}{\tau^2} = \left(\rho_4 / \langle r^4 \rangle_{HF}\right)^{1/2} \quad , \tag{13}$$

and from equation (12) for $n = 2$, we obtain

$$\rho_2 = \langle r^2 \rangle_{HF} \left(\rho_4 / \langle r^4 \rangle_{HF}\right)^{1/2} \quad , \tag{14}$$

which can be used to obtain theoretical values of $B_{2m}$ by equation (6). The $\rho_2$ and $\rho_4$ determined by equations (14) and (11) were used in equation (6) to determine values of the crystal field parameter for $Cr^{3+}$. These values of $B_{nm}$ along with the $F^{(k)}$ of table 8 and with $\zeta = 220\ cm^{-1}$ (80 percent of the free ion value) were used to calculate the ground-state splitting (0.53 $cm^{-1}$) and the splitting of the $^2E$ level (19.6 $cm^{-1}$). Both of these calculated splittings were much too large. Consequently, the value of $B_{20}$ was varied to obtain a best fit to these splittings, and a value of $B_{20} = 2832\ cm^{-1}$ was found, which is approximately 0.5301 times the value given by equation (14). Thus all the values of $\rho_2$ given by equation (14) were multiplied by 0.5301. The values of $\rho_4$ were obtained from equation (11) and these values are given in table 16 for the triply ionized $3d^N$ transition metal ion series. In obtaining these results, we used the Hartree-Fock values of $\langle r^n \rangle$ given by Fraga et al [18]. Further, the results obtained from the experimental values of $\rho_4$ were linear least-squares fit to obtain values of $\rho_2$ and $\rho_4$ for ions not reported.

The values of $\rho_2$ and $\rho_4$ given in table 16 were used in equation (6) to obtain crystal field parameters $B_{nm}$ which were used (fixed) to fit the experimental data given in tables 2 through 12 with $F^{(2)}$ and $F^{(4)}$ varying. The resulting $F^{(2)}$ and $F^{(4)}$ were linear least-squares fit, and the final $F^{(k)}$ and $B_{nm}$ are given in table 17. Since most of the experimental data are analyzed in terms of Racah parameters $B$ and $C$, as well as various crystal field parameters, two sets of these parameters (Macfarlane's [19] and Bellhauser's [20]) are given in table 18.

The set of parameters given in table 17, along with the spin-orbit coupling set at 80 percent of the free ion value [21] and $\alpha = 30\ cm^{-1}$, was used to calculate the energy levels for the $3d^1$ through the $3d^9$ ions. The results are given in tables 19 through 27.

**Table 13. Crystallographic data on $Y_3Al_5O_{12}$**

*[Cubic $O_h^{10}$ (Ia3d) No. 230, z = 8]*

| Ion | Site | Symm | x[a] | y | z | q | α(Å$^3$)[b] |
|---|---|---|---|---|---|---|---|
| $Al_1$ | 16(a) | $C_{3i}$ | 0 | 0 | 0 | 3 | 0.0530 |
| $Al_2$ | 24(d) | $S_4$ | 0 | 1/4 | 3/8 | 3 | 0.0530 |
| Y | 24(c) | $D_2$ | 0 | 1/4 | 1/8 | 3 | 0.870 |
| O | 96(h) | $C_1$ | –0.0306 | –0.0512 | 0.1500 | –2 | 1.349 |

[a] *X-ray data, a = 12.000 Å, reference 14.*

[b] *Taken from reference 15.*

**Table 14. Lattice sum, $A_{nm}$ ($cm^{-1}/Å^n$), for $Al_2$ ion in 24($d$) ($S_4$) site in $Y_3Al_5O_{12}$**

| $A_{nm}$ | Point charge | Self–induced | Dipole | Total |
|---|---|---|---|---|
| $A_{20}$ | 6,355 | –2,604 | 14,013 | 17,765 |
| $ReA_{32}$ | –27,522 | 8,609 | –11,957 | –30,870 |
| $ImA_{32}$ | 37,839 | –11,913 | 6,332 | 32,258 |
| $A_{40}$ | –25,089 | 11,879 | –8,516 | –21,726 |
| $ReA_{44}$ | –3,763 | 1,614 | 1,964 | –185.1 |
| $ImA_{44}$ | –9,108 | 4,740 | –2,875 | –7,243 |
| $ReA_{52}$ | –2,931 | 2,287 | –3,498 | –4,142 |
| $ImA_{52}$ | 4,328 | –3,207 | 3,640 | 4,762 |
| $\|A_{44}\|$ | 9,855 | — | — | 7,245 |

**Table 15. Lattice sum, $A_{nm}$ ($cm^{-1}/Å^n$), for $Al_1$ ion in 16($a$) ($C_{3i}$) site in $Y_3Al_5O_{12}$**

***[Rotated so that the z-axis is parallel to the (111) crystallographic axis]***

| $A_{nm}$ | Point charge | Self–induced | Dipole | Total |
|---|---|---|---|---|
| $A_{20}$ | 6,836 | –1,107 | –13,553 | –7,823 |
| $A_{40}$ | –20,054 | 8,166 | 3,273 | –8,615 |
| $ReA_{43}$ | 2,813 | –1,422 | 6,253 | 7,644 |
| $ImA_{43}$ | –22,370 | 8,639 | 2,348 | –11,383 |
| $\|A_{43}\|$ | 22,546 | — | — | 13,711 |

**Table 16. Linear least-squares best fit values of $\rho_2$ and $\rho_4$ for triply ionized transition metal ions in octahedral ($C_{3i}$) site in YAG**

| Ion | $3d^N$ | $\rho_2(Å^2)$ | $\rho_4(Å^4)$ |
|---|---|---|---|
| Ti | $d^1$ | 0.4301 | 1.3431 |
| V | $d^2$ | 0.4234 | 1.3039 |
| Cr | $d^3$ | 0.4142 | 1.2647 |
| Mn | $d^4$ | 0.4050 | 1.2255 |
| Fe | $d^5$ | 0.3963 | 1.1864 |
| Co | $d^6$ | 0.3855 | 1.1472 |
| Ni | $d^7$ | 0.3756 | 1.1080 |
| Cu | $d^8$ | 0.3660 | 1.0689 |
| Zn | $d^9$ | 0.3567 | 1.0297 |

**Table 17. Linear least-squares best fit values of $F^{(k)}$ ($cm^{-1}$) and $B_{nm}$($cm^{-1}$) for triply ionized transition metal ions in the octahedral site ($C_{3i}$) in YAG**

| Ion | $3d^N$ | $F^{(2)}$ | $F^{(4)}$ | $B_{20}$ | $B_{40}$ | $B_{43}$ |
|---|---|---|---|---|---|---|
| Ti | $d^1$ | — | — | 2953 | –26934 | 30280 |
| V | $d^2$ | 56732 | 36132 | 2895 | –26148 | 29397 |
| Cr | $d^3$ | 59983 | 38912 | 2832 | –25363 | 28514 |
| Mn | $d^4$ | 63234 | 41688 | 2769 | –24577 | 27631 |
| Fe | $d^5$ | 66485 | 44463 | 2709 | –23792 | 26748 |
| Co | $d^6$ | 69736 | 47239 | 2635 | –23006 | 25865 |
| Ni | $d^7$ | 72987 | 50015 | 2568 | –22221 | 24982 |
| Cu | $d^8$ | 76238 | 52790 | 2502 | –21435 | 24099 |
| Zn | $d^9$ | — | — | 2438 | –20650 | 23216 |

**Table 18. Racah parameters, $B$ and $C$; Macfarlane's parameters, $Dq$, v, and v′; and Ballhausen's parameters, $Dq$, $D\sigma$, and $D\tau$, for triply ionized transition metal ions in octahedral ($C_{3i}$) site in YAG.**

| Ion | $3d^N$ | $B$ | $C$ | $Dq^{(a)}$ | v | v′ | $Dq^{(b)}$ | $D\sigma$ | $D\tau$ |
|---|---|---|---|---|---|---|---|---|---|
| Ti | $d^1$ | — | — | 1839 | 758.0 | –776.1 | 1810 | –421.9 | 76.15 |
| V | $d^2$ | 748.1 | 2868 | 1786 | 747.7 | –759.0 | 1757 | –413.5 | 73.93 |
| Cr | $d^3$ | 783.0 | 3088 | 1732 | 735.5 | –741.1 | 1704 | –404.5 | 71.71 |
| Mn | $d^4$ | 817.8 | 3309 | 1678 | 723.3 | –723.3 | 1651 | –395.5 | 69.49 |
| Fe | $d^5$ | 852.7 | 3529 | 1625 | 712.7 | –705.9 | 1599 | –387.0 | 67.27 |
| Co | $d^6$ | 887.6 | 3749 | 1571 | 695.8 | –685.7 | 1546 | –376.5 | 65.04 |
| Ni | $d^7$ | 922.5 | 3969 | 1517 | 681.6 | –666.8 | 1493 | –366.8 | 62.82 |
| Cu | $d^8$ | 957.3 | 4190 | 1464 | 668.3 | –648.3 | 1441 | –357.4 | 60.60 |
| Zn | $d^9$ | — | — | 1410 | 655.8 | –630.2 | 1387 | –348.3 | 58.38 |

[a]*Reference 19.* [b]*Reference 20.*

**Table 19. Energy levels ($cm^{-1}$) of $Ti^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 122.24$ ($cm^{-1}$)**

| Level No. | IR[a] | Energy | Free-ion state (%) |
|---|---|---|---|
| 1 | 6 | 0 | 100 2D |
| 2 | 4,5 | 128 | 100 2D |
| 3 | 4,5 | 868 | 100 2D |
| 4 | 4,5 | 18773 | 100 2D |
| 5 | 6 | 18787 | 100 2D |

[a] *4,5 and 6 are abbreviations for the $\Gamma_{4,5}$ and $\Gamma_6$ irreducible representations of the $C_{3i}$ double group. Levels labeled 6 are also doublets.*

**Table 20. Energy levels ($cm^{-1}$) of $V^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 164.80$ ($cm^{-1}$)**

| Level No. | IR[a] | Energy | Free-ion state (%) |
|---|---|---|---|
| 1 | 1 | 0 | 90 3F + 10 3P |
| 2 | 2,3 | 13 | 90 3F + 10 3P |
| 3 | 2,3 | 156 | 93 3F + 7 3P |
| 4 | 2,3 | 313 | 92 3F + 8 3P |
| 5 | 1 | 386 | 93 3F + 7 3P |
| 6 | 1 | 441 | 92 3F + 8 3P |
| 7 | 2,3 | 10582 | 54 1D + 46 1G |
| 8 | 1 | 11086 | 62 1D + 37 1G |
| 9 | 2,3 | 11181 | 54 1D + 46 1G |
| 10 | 1 | 16405 | 100 3F |
| 11 | 2,3 | 16413 | 100 3F |
| 12 | 1 | 16734 | 100 3F |
| 13 | 1 | 16737 | 100 3F |
| 14 | 2,3 | 16783 | 100 3F |
| 15 | 2,3 | 16826 | 100 3F |
| 16 | 1 | 23377 | 68 1G + 31 1S |
| 17 | 1 | 25453 | 88 3P + 12 3F |
| 18 | 2,3 | 25456 | 88 3P + 12 3F |
| 19 | 1 | 26436 | 92 3P + 8 3F |
| 20 | 1 | 26447 | 92 3P + 7 3F |
| 21 | 2,3 | 26504 | 93 3P + 7 3F |
| 22 | 2,3 | 26565 | 93 3P + 7 3F |
| 23 | 2,3 | 28764 | 57 1G + 43 1D |
| 24 | 1 | 28805 | 62 1G + 37 1D |
| 25 | 1 | 31367 | 100 1G |
| 26 | 2,3 | 31837 | 99 1G + 1 1D |
| 27 | 1 | 34650 | 99 3F + 1 3P |
| 28 | 2,3 | 34651 | 99 3F + 1 3P |
| 29 | 1 | 46539 | 51 1G + 49 1D |
| 30 | 2,3 | 61136 | 69 1S + 31 1G |

[a] *Labels 1 and 2,3 are abbreviations for the $\Gamma_1$ and $\Gamma_{2,3}$ irreducible representations of the $C_{3i}$ group.*

**Table 21. Energy levels ($cm^{-1}$) of $Cr^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 220.00$ ($cm^{-1}$)**

| Level No. | IR[a] | Energy | Free ion state (%) | Level No. | IR[a] | Energy | Free ion state (%) |
|---|---|---|---|---|---|---|---|
| 1 | 4,5 | 0 | 100 4F | 31 | 4,5 | 34715 | 50 2H + 38 2D2 + 10 2D1 |
| 2 | 6 | 0 | 100 4F | 32 | 4,5 | 37935 | 29 2H + 20 4F + 20 4P |
| 3 | 4,5 | 15099 | 61 2G + 19 2H + 17 2D2 | 33 | 6 | 38024 | 28 4P + 27 4F + 19 2H |
| 4 | 6 | 15119 | 61 2G + 19 2H + 17 2D2 | 34 | 4,5 | 38036 | 23 2H + 22 4F + 22 4P |
| 5 | 6 | 15788 | 41 2G + 34 2H + 20 2P | 35 | 4,5 | 38130 | 52 4P + 48 4F |
| 6 | 4,5 | 15816 | 40 2G + 34 2H + 21 2P | 36 | 4,5 | 38273 | 32 4P + 32 4F + 14 2H |
| 7 | 4,5 | 16062 | 38 2G + 32 2H + 23 2P | 37 | 6 | 38311 | 24 4P + 22 4F + 21 2H |
| 8 | 4,5 | 17163 | 100 4F | 38 | 4,5 | 38381 | 27 4P + 26 4F + 18 2H |
| 9 | 4,5 | 17205 | 99 4F + 1 2G | 39 | 4,5 | 39898 | 58 4P + 41 4F |
| 10 | 6 | 17250 | 99 4F + 1 2G | 40 | 6 | 39916 | 58 4P + 41 4F + 1 2P |
| 11 | 4,5 | 17307 | 98 4F + 1 2G | 41 | 4,5 | 43545 | 56 2F + 40 2D2 + 2 2G |
| 12 | 6 | 17630 | 99 4F + 1 2G | 42 | 6 | 43586 | 56 2F + 40 2D2 + 2 2G |
| 13 | 4,5 | 17637 | 99 4F + 1 2G | 43 | 4,5 | 43768 | 63 2F + 35 2D2 + 1 2G |
| 14 | 4,5 | 22114 | 30 2H + 29 2D1 + 20 2D2 | 44 | 4,5 | 45378 | 99 2F |
| 15 | 6 | 22750 | 35 2H + 28 2D1 + 18 2D2 | 45 | 4,5 | 49752 | 65 2H + 33 2G + 2 2D2 |
| 16 | 4,5 | 22846 | 35 2H + 28 2D1 + 18 2D2 | 46 | 6 | 49843 | 64 2H + 33 2G + 1 2D2 |
| 17 | 4,5 | 24405 | 58 4F + 41 4P | 47 | 4,5 | 50494 | 69 2H + 29 2G + 1 2P |
| 18 | 6 | 24408 | 58 4F + 41 4P | 48 | 4,5 | 51132 | 30 2G + 22 2H + 19 2F |
| 19 | 4,5 | 24999 | 52 4F + 47 4P | 49 | 4,5 | 51728 | 27 2H + 26 2G + 21 2F |
| 20 | 6 | 25012 | 51 4F + 48 4P | 50 | 6 | 51817 | 26 2G + 26 2H + 22 2F |
| 21 | 4,5 | 25025 | 51 4F + 49 4P | 51 | 4,5 | 54078 | 41 2D2 + 22 2D1 + 22 2G |
| 22 | 4,5 | 25036 | 50 4F + 50 4P | 52 | 6 | 54090 | 41 2D2 + 22 2D1 + 22 2G |
| 23 | 4,5 | 29991 | 100 2G | 53 | 4,5 | 57404 | 69 2F + 23 2P + 7 2H |
| 24 | 4,5 | 32345 | 57 2G + 37 2H + 4 2D2 | 54 | 6 | 57410 | 68 2F + 24 2P + 7 2H |
| 25 | 6 | 32378 | 58 2G + 36 2H + 4 2D2 | 55 | 4,5 | 57542 | 69 2F + 24 2P + 6 2H |
| 26 | 4,5 | 32662 | 46 2H + 30 2G + 23 2P | 56 | 6 | 72614 | 60 2D1 + 19 2D2 + 14 2F |
| 27 | 4,5 | 32823 | 52 2G + 44 2H + 3 2D2 | 57 | 4,5 | 72734 | 60 2D1 + 19 2D2 + 14 2F |
| 28 | 4,5 | 32975 | 50 2H + 28 2G + 19 2P | 58 | 4,5 | 73980 | 60 2D1 + 23 2D2 + 13 2F |
| 29 | 6 | 33077 | 50 2H + 25 2G + 21 2P | 59 | 6 | 74606 | 64 2D1 + 17 2H + 14 2G |
| 30 | 6 | 34709 | 49 2H + 38 2D2 + 10 2D1 | 60 | 4,5 | 74642 | 64 2D1 + 17 2H + 14 2G |

[a] *Labels 4,5 and 6 are abbreviations for the $\Gamma_{4,5}$ and $\Gamma_6$ irreducible representations of the $C_{3i}$ double group. Levels labeled 6 are aslo doublets.*

**Table 22. Energy levels ($cm^{-1}$) of $Mn^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 289.44$ ($cm^{-1}$)**

| Level No. | IR[a] | Energy | Free ion state (%) |
|---|---|---|---|
| 1 | 1 | 0 | 99 5D |
| 2 | 2,3 | 12 | 99 5D |
| 3 | 1 | 24 | 99 5D |
| 4 | 2,3 | 35 | 99 5D |
| 5 | 2,3 | 50 | 100 5D |
| 6 | 1 | 60 | 100 5D |
| 7 | 1 | 66 | 100 5D |
| 8 | 1 | 3295 | 38 3H + 18 3G + 15 3F1 |
| 9 | 1 | 3354 | 39 3H + 18 3G + 15 3F1 |
| 10 | 2,3 | 3455 | 39 3H + 17 3G + 15 3F1 |
| 11 | 2,3 | 3614 | 41 3H + 17 3G + 15 3F1 |
| 12 | 2,3 | 3918 | 41 3H + 15 3G + 14 3F1 |
| 13 | 1 | 3921 | 41 3H + 15 3G + 14 3F1 |
| 14 | 1 | 12948 | 32 1I + 30 1G2 + 23 1G1 |
| 15 | 2,3 | 13108 | 35 1I + 28 1G2 + 23 1G1 |
| 16 | 2,3 | 14297 | 59 1I + 20 1D2 + 10 1G1 |
| 17 | 1 | 16316 | 98 5D + 1 3H |
| 18 | 2,3 | 16324 | 98 5D + 1 3H |
| 19 | 2,3 | 16347 | 99 5D |
| 20 | 1 | 16936 | 97 5D + 1 3H + 1 3P2 |
| 21 | 1 | 16936 | 97 5D + 1 3H + 1 3P2 |
| 22 | 2,3 | 17031 | 97 5D + 1 3H + 1 3F2 |
| 23 | 2,3 | 17114 | 97 5D + 1 3H + 1 3F2 |
| 24 | 1 | 17173 | 97 5D + 1 3F2 + 1 3H |
| 25 | 1 | 17205 | 97 5D + 1 3F2 + 1 3H |
| 26 | 2,3 | 17260 | 97 5D + 1 3F2 + 1 3H |
| 27 | 2,3 | 18031 | 84 3H + 14 3G + 1 3D |
| 28 | 2,3 | 18049 | 84 3H + 14 3G + 1 3D |
| 29 | 1 | 18051 | 84 3H + 14 3G + 1 3D |
| 30 | 1 | 18061 | 84 3H + 14 3G + 1 3D |
| 31 | 1 | 18344 | 46 3H + 20 3G + 17 3P2 |
| 32 | 2,3 | 18402 | 45 3H + 22 3G + 17 3P2 |
| 33 | 1 | 18640 | 46 3H + 19 3P2 + 18 3G |
| 34 | 1 | 18742 | 45 3H + 21 3G + 19 3P2 |
| 35 | 2,3 | 18799 | 45 3H + 20 3G + 19 3P2 |
| 36 | 2,3 | 18879 | 44 3H + 20 3G + 19 3P2 |
| 37 | 2,3 | 19273 | 38 3F2 + 32 3H + 13 3F1 |
| 38 | 2,3 | 19333 | 40 3F2 + 3i 3H + 13 3F1 |
| 39 | 1 | 19379 | 40 3F2 + 32 3H + 13 3F1 |
| 40 | 1 | 19424 | 41 3F2 + 32 3H + 13 3F1 |
| 41 | 2,3 | 19650 | 40 3F2 + 32 3H + 12 3F1 |
| 42 | 1 | 19662 | 41 3F2 + 32 3H + 12 3F1 |
| 43 | 2,3 | 21132 | 93 3G + 4 3F2 + 1 3H |
| 44 | 1 | 21137 | 95 3G + 3 3F2 + 1 3H |
| 45 | 1 | 21140 | 33 1G1 + 23 1I + 23 1S2 |
| 46 | 1 | 21370 | 91 3F2 + 7 3F1 + 1 5D |
| 47 | 2,3 | 21376 | 90 3F2 + 7 3F1 + 1 3G |
| 48 | 1 | 24200 | 52 3D + 44 3G + 4 3H |
| 49 | 2,3 | 24201 | 52 3D + 44 3G + 4 3H |
| 50 | 1 | 24202 | 52 3D + 44 3G + 4 3H |
| 51 | 2,3 | 24204 | 52 3D + 44 3G + 4 3H |
| 52 | 2,3 | 27088 | 60 1I + 23 1G2 + 8 1G1 |
| 53 | 1 | 27310 | 64 1I + 21 1G2 + 7 1G1 |
| 54 | 1 | 27328 | 92 1I + 8 1F |
| 55 | 1 | 28890 | 40 1I + 24 1G2 + 20 1G1 |
| 56 | 2,3 | 29238 | 39 1I + 26 1G2 + 20 1G1 |
| 57 | 2,3 | 30403 | 39 3G + 30 3H + 19 3P1 |
| 58 | 2,3 | 30440 | 39 3G + 29 3H + 19 3P1 |
| 59 | 1 | 30467 | 40 3G + 29 3H + 18 3P1 |
| 60 | 1 | 30[illegible] | 41 3G + 28 3H + 18 3P1 |
| 61 | 2,3 | 30797 | 43 3G + 27 3H + 19 3P1 |
| 62 | 1 | 30799 | 44 3G + 28 3H + 19 3P1 |
| 63 | 2,3 | 31190 | 41 1D2 + 32 1G2 + 16 1I |
| 64 | 1 | 32618 | 33 3D + 26 3G + 24 3F1 |
| 65 | 1 | 32645 | 32 3D + 26 3G + 24 3F1 |
| 66 | 2,3 | 32656 | 31 3D + 27 3G + 23 3F1 |
| 67 | 2,3 | 32682 | 29 3D + 28 3G + 23 3F1 |
| 68 | 2,3 | 32819 | 33 3G + 31 3D + 24 3F1 |
| 69 | 1 | 32821 | 33 3G + 31 3D + 24 3F1 |
| 70 | 1 | 34849 | 48 3H + 32 3F2 + 6 3G |
| 71 | 1 | 34873 | 48 3H + 33 3F2 + 5 3G |
| 72 | 2,3 | 34905 | 47 3H + 33 3F2 + 6 3F1 |
| 73 | 2,3 | 34944 | 47 3H + 33 3F2 + 6 3F1 |
| 74 | 1 | 35176 | 51 3H + 30 3F2 + 6 3F1 |
| 75 | 2,3 | 35182 | 50 3H + 29 3F2 + 6 3F1 |
| 76 | 1 | 3667[illegible] | 49 3H + 25 3F2 + 18 3D |
| 77 | 2,3 | 366[illegible] | 49 3H + 26 3F2 + 18 3D |
| 78 | 1 | 37256 | 46 3H + 28 3D + 16 3F2 |
| 79 | 1 | 37264 | 45 3H + 28 3D + 16 3F2 |
| 80 | 2,3 | 37274 | 45 3H + 29 3D + 17 3F2 |
| 81 | 2,3 | 37297 | 44 3H + 30 3D + 17 3F2 |
| 82 | 2,3 | 39307 | 45 3D + 41 3G + 11 3H |
| 83 | 1 | 39310 | 46 3D + 41 3G + 11 3H |
| 84 | 2,3 | 39313 | 46 3D + 41 3G + 11 3H |
| 85 | 1 | 39316 | 46 3D + 41 3G + 11 3H |
| 86 | 1 | 40104 | 47 3G + 34 3F2 + 15 3D |

**Table 22. Energy levels ($cm^{-1}$) of $Mn^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 289.44$ ($cm^{-1}$) (cont'd)**

| Level No. | IR[a] | Energy | Free ion state (%) | Level No. | IR[a] | Energy | Free ion state (%) |
|---|---|---|---|---|---|---|---|
| 87 | 1 | 40146 | 46 3G + 34 3F2 + 15 3D | 115 | 1 | 54639 | 68 3F1 + 18 3H + 9 3P1 |
| 88 | 2,3 | 40226 | 46 3G + 33 3F2 + 16 3D | 116 | 2,3 | 55026 | 72 3F1 + 18 3H + 5 3P1 |
| 89 | 2,3 | 40378 | 46 3G + 33 3F2 + 17 3D | 117 | 1 | 55055 | 72 3F1 + 17 3H + 5 3P1 |
| 90 | 2,3 | 40681 | 44 3G + 27 3D + 26 3F2 | 118 | 1 | 58711 | 91 3F1 + 8 3F2 |
| 91 | 1 | 40701 | 44 3G + 28 3D + 26 3F2 | 119 | 2,3 | 58711 | 91 3F1 + 8 3F2 |
| 92 | 1 | 41720 | 38 1G2 + 23 1S2 + 19 1I | 120 | 1 | 61623 | 50 3P1 + 22 3F2 + 16 3P2 |
| 93 | 2,3 | 42473 | 41 1F + 23 1I + 17 1G1 | 121 | 2,3 | 61627 | 50 3P1 + 22 3F2 + 16 3P2 |
| 94 | 1 | 42813 | 83 1I + 6 1G2 + 3 1D1 | 122 | 2,3 | 62141 | 44 3P1 + 24 3F2 + 12 3F1 |
| 95 | 2,3 | 43437 | 78 1I + 8 1G2 + 5 1F | 123 | 2,3 | 62260 | 44 3P1 + 23 3F2 + 12 3P2 |
| 96 | 1 | 43446 | 40 1F + 19 1I + 18 1G2 | 124 | 1 | 62342 | 44 3P1 + 23 3F2 + 12 3P2 |
| 97 | 1 | 43537 | 51 3P2 + 22 3F2 + 12 3G | 125 | 1 | 62385 | 44 3P1 + 22 3F2 + 13 3P2 |
| 98 | 1 | 43565 | 49 3P2 + 20 3F2 + 12 3G | 126 | 2,3 | 63350 | 62 1G1 + 24 1G2 + 8 1D2 |
| 99 | 2,3 | 43603 | 46 3P2 + 19 3F2 + 11 3G | 127 | 1 | 64278 | 63 1G1 + 36 1I + 1 1F |
| 100 | 2,3 | 43706 | 45 3P2 + 17 3F2 + 11 3G | 128 | 1 | 64891 | 59 3F1 + 16 3D + 15 3G |
| 101 | 2,3 | 43867 | 22 1F + 19 3P2 + 14 1G2 | 129 | 2,3 | 64892 | 58 3F1 + 16 3D + 14 3G |
| 102 | 2,3 | 43905 | 40 1F + 11 1G1 + 10 3P2 | 130 | 2,3 | 65357 | 60 1G1 + 34 1I + 2 1F |
| 103 | 1 | 43983 | 49 1F + 12 3P2 + 10 1G1 | 131 | 2,3 | 66284 | 54 3F1 + 15 3D + 15 3G |
| 104 | 1 | 44088 | 42 3P2 + 20 3F2 + 13 1F | 132 | 2,3 | 66292 | 54 3F1 + 15 3D + 14 3G |
| 105 | 2,3 | 44116 | 40 3P2 + 19 3F2 + 10 1G2 | 133 | 1 | 66299 | 53 3F1 + 16 3D + 14 3G |
| 106 | 1 | 46037 | 41 1G2 + 27 1I + 18 1S2 | 134 | 1 | 66306 | 54 3F1 + 16 3D + 14 3G |
| 107 | 2,3 | 51578 | 61 1D2 + 10 1I + 9 1G1 | 135 | 2,3 | 72473 | 37 1G1 + 27 1G2 + 19 1D2 |
| 108 | 1 | 51653 | 71 1D2 + 9 1I + 9 1G1 | 136 | 1 | 73177 | 37 1G1 + 24 1G2 + 15 1D2 |
| 109 | 1 | 52486 | 81 1F + 11 1G2 + 7 1I | 137 | 1 | 75774 | 34 1G1 + 24 1I + 18 1S2 |
| 110 | 2,3 | 53409 | 49 1G2 + 38 1F + 6 1D2 | 138 | 1 | 78667 | 54 1D1 + 18 1F + 12 1G1 |
| 111 | 1 | 53533 | 52 1F + 45 1G2 + 3 1I | 139 | 2,3 | 81044 | 57 1D1 + 18 1F + 10 1G2 |
| 112 | 2,3 | 54472 | 68 3F1 + 18 3H + 10 3P1 | 140 | 2,3 | 82543 | 77 1D1 + 20 1D2 + 1 1G2 |
| 113 | 2,3 | 54537 | 68 3F1 + 18 3H + 9 3P1 | 141 | 1 | 102454 | 73 1S1 + 13 1G1 + 11 1S2 |
| 114 | 1 | 54606 | 68 3F1 + 18 3H + 9 3P1 | | | | |

[a] *Labels 1 and 2,3 are abbreviations for the $\Gamma_1$ and $\Gamma_{2,3}$ irreducible representations of the $C_{3i}$ group.*

**Table 23. Energy levels ($cm^{-1}$) of $Fe^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 370.40$ ($cm^{-1}$)**

| Level No. | IR[a] | Energy | Free ion state (%) |
|---|---|---|---|
| 1 | 4,5 | 0.00 | 100 6S |
| 2 | 6 | 0.187 | 100 6S |
| 3 | 4,5 | 0.262 | 100 6S |
| 4 | 4,5 | 12196 | 21 4G + 18 2I + 16 2H |
| 5 | 4,5 | 12725 | 38 4G + 26 4P + 9 2I |
| 6 | 6 | 12729 | 38 4G + 26 4P + 10 2I |
| 7 | 6 | 13046 | 57 4G + 38 4P + 4 4F |
| 8 | 4,5 | 13105 | 57 4G + 39 4P + 3 4F |
| 9 | 4,5 | 13156 | 57 4G + 39 4P + 3 4F |
| 10 | 4,5 | 13480 | 37 4G + 25 4P + 11 2I |
| 11 | 6 | 13608 | 20 2I + 20 4G + 18 2H |
| 12 | 4,5 | 13618 | 20 4G + 20 2I + 17 2H |
| 13 | 4,5 | 18323 | 50 4G + 28 4F + 21 4D |
| 14 | 6 | 18336 | 50 4G + 28 4F + 21 4D |
| 15 | 4,5 | 18861 | 47 4G + 28 4F + 25 4D |
| 16 | 6 | 18871 | 48 4G + 28 4F + 24 4D |
| 17 | 4,5 | 18872 | 49 4G + 28 4F + 23 4D |
| 18 | 4,5 | 18884 | 49 4G + 28 4F + 23 4D |
| 19 | 4,5 | 25784 | 52 2I + 39 2F1 + 3 2F2 |
| 20 | 4,5 | 25958 | 46 2I + 18 2H + 17 4G |
| 21 | 6 | 25990 | 45 2I + 22 4G + 19 2H |
| 22 | 4,5 | 26314 | 40 2I + 29 4G + 17 2H |
| 23 | 4,5 | 26633 | 89 4G + 5 2I + 3 2F1 |
| 24 | 4,5 | 26723 | 95 4G + 2 2I + 1 2F1 |
| 25 | 6 | 26737 | 95 4G + 2 2I + 1 2F1 |
| 26 | 4,5 | 26956 | 78 4G + 13 2I + 5 2H |
| 27 | 4,5 | 26982 | 73 4G + 17 2I + 6 2H |
| 28 | 6 | 26986 | 78 4G + 14 2I + 5 2H |
| 29 | 4,5 | 27891 | 46 2I + 23 2F1 + 11 2H |
| 30 | 6 | 28000 | 45 2I + 23 2F1 + 12 2H |
| 31 | 4,5 | 28003 | 43 2I + 21 2F1 + 12 2H |
| 32 | 4,5 | 29247 | 43 4D + 35 4G + 6 2H |
| 33 | 6 | 29289 | 43 4D + 34 4G + 7 2H |
| 34 | 4,5 | 29418 | 52 4D + 41 4G + 3 4F |
| 35 | 4,5 | 29554 | 56 4D + 41 4G + 3 4F |
| 36 | 6 | 29686 | 40 4D + 27 4G + 10 2I |
| 37 | 4,5 | 29829 | 38 4D + 25 4G + 11 2I |
| 38 | 4,5 | 29912 | 33 4D + 22 4G + 14 2I |
| 39 | 6 | 29935 | 29 4D + 20 4G + 16 2I |
| 40 | 4,5 | 32302 | 99 4D |
| 41 | 6 | 32303 | 99 4D |
| 42 | 4,5 | 32307 | 99 4D |
| 43 | 4,5 | 32313 | 99 4D |
| 44 | 6 | 34446 | 30 2G2 + 24 2F1 + 21 2H |
| 45 | 4,5 | 34478 | 29 2G2 + 23 2F1 + 21 2H |
| 46 | 4,5 | 34972 | 30 2G2 + 23 2F1 + 20 2H |
| 47 | 4,5 | 37052 | 35 2I + 23 2G2 + 14 2F2 |
| 48 | 4,5 | 37848 | 49 2I + 20 2G2 + 10 2F2 |
| 49 | 6 | 37898 | 29 2G2 + 23 2F2 + 19 2I |
| 50 | 4,5 | 37950 | 30 2I + 28 2G2 + 17 2F2 |
| 51 | 6 | 38553 | 28 4P + 24 4F + 19 2I |
| 52 | 4,5 | 38634 | 33 4P + 28 4F + 14 2I |
| 53 | 4,5 | 38949 | 30 2I + 18 4P + 16 4F |
| 54 | 6 | 39088 | 25 2I + 22 4P + 19 4F |
| 55 | 4,5 | 39657 | 39 4P + 38 4F + 14 4G |
| 56 | 6 | 39802 | 37 4P + 36 4F + 14 4G |
| 57 | 4,5 | 39848 | 39 4P + 39 4F + 15 4G |
| 58 | 4,5 | 39900 | 38 4P + 37 4F + 14 4G |
| 59 | 4,5 | 40763 | 47 2I + 35 2D3 + 9 2D1 |
| 60 | 6 | 40814 | 45 2I + 35 2D3 + 9 2D1 |
| 61 | 4,5 | 40869 | 41 2I + 34 2D3 + 9 2D1 |
| 62 | 4,5 | 41825 | 52 2G2 + 22 2I + 14 2G1 |
| 63 | 4,5 | 43883 | 99 4F |
| 64 | 6 | 43887 | 99 4F |
| 65 | 6 | 45110 | 68 2G2 + 10 2I + 5 2H |
| 66 | 4,5 | 45176 | 70 2G2 + 10 2I + 5 2D3 |
| 67 | 4,5 | 46241 | 60 2H + 28 2F1 + 5 2G2 |
| 68 | 4,5 | 46325 | 55 2H + 22 2F1 + 11 2F2 |
| 69 | 6 | 46373 | 42 2H + 18 2F2 + 17 2F1 |
| 70 | 6 | 46735 | 26 2F2 + 22 2H + 18 2G2 |
| 71 | 4,5 | 46883 | 34 2F2 + 20 2G2 + 14 2H |
| 72 | 4,5 | 47324 | 48 2F2 + 22 2G2 + 15 2I |
| 73 | 4,5 | 47617 | 51 2F2 + 20 2I + 19 2G2 |
| 74 | 4,5 | 48403 | 33 2F2 + 28 2G2 + 16 4F |
| 75 | 4,5 | 48445 | 40 4F + 19 4G + 13 4P |
| 76 | 6 | 48533 | 40 2F2 + 37 2G2 + 7 2I |
| 77 | 4,5 | 48542 | 37 2F2 + 19 4F + 14 2G2 |
| 78 | 4,5 | 48565 | 34 4F + 19 2F2 + 17 4G |
| 79 | 6 | 48674 | 49 4F + 24 4G + 16 4P |
| 80 | 4,5 | 48813 | 53 4F + 26 4G + 17 4P |
| 81 | 6 | 49682 | 56 4F + 27 4G + 15 4P |
| 82 | 4,5 | 49730 | 55 4F + 26 4G + 15 4P |
| 83 | 4,5 | 52620 | 69 2S + 24 2G2 + 5 2G1 |
| 84 | 6 | 53040 | 42 2H + 30 2D3 + 22 2D2 |
| 85 | 4,5 | 53069 | 42 2H + 30 2D3 + 22 2D2 |
| 86 | 4,5 | 54048 | 31 2H + 22 2F2 + 18 2F1 |

**Table 23. Energy levels ($cm^{-1}$) of $Fe^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 370.40$ ($cm^{-1}$) (cont'd)**

| Level No. | IR[a] | Energy | Free ion state (%) |
|---|---|---|---|
| 87 | 4,5 | 54476 | 65 4F + 19 4D + 10 4G |
| 88 | 4,5 | 54514 | 63 4F + 19 4D + 9 4G |
| 89 | 6 | 54575 | 61 4F + 18 4D + 9 4G |
| 90 | 4,5 | 54731 | 49 4F + 16 4D + 10 2H |
| 91 | 6 | 54923 | 59 4F + 18 4D + 9 4G |
| 92 | 4,5 | 54981 | 65 4F + 20 4D + 10 4G |
| 93 | 6 | 55138 | 29 2H + 21 2F2 + 14 2F1 |
| 94 | 4,5 | 55154 | 25 2H + 20 4F + 18 2F2 |
| 95 | 4,5 | 55831 | 28 2F1 + 19 2H + 17 2G2 |
| 96 | 6 | 55938 | 27 2F1 + 18 2G2 + 17 2H |
| 97 | 4,5 | 56215 | 29 2F1 + 18 2H + 17 2G2 |
| 98 | 4,5 | 59435 | 41 2H + 30 2I + 17 2F1 |
| 99 | 6 | 59620 | 42 2H + 30 2I + 16 2F1 |
| 100 | 4,5 | 59912 | 41 2F1 + 25 2I + 24 2F2 |
| 101 | 4,5 | 60505 | 34 2H + 25 2I + 20 2F1 |
| 102 | 4,5 | 64728 | 60 2G1 + 10 2H + 9 2D1 |
| 103 | 6 | 64792 | 60 2G1 + 10 2H + 9 2D1 |
| 104 | 4,5 | 66844 | 62 2D2 + 12 2G1 + 9 2F2 |
| 105 | 6 | 67257 | 51 2D2 + 22 2G1 + 10 2I |
| 106 | 4,5 | 67316 | 51 2D2 + 22 2G1 + 10 2I |
| 107 | 4,5 | 68429 | 51 2D2 + 16 2G1 + 9 2G2 |
| 108 | 6 | 68481 | 47 2D2 + 16 2G1 + 11 2H |
| 109 | 4,5 | 69067 | 31 2H + 22 2D3 + 18 2I |
| 110 | 6 | 69666 | 21 2D3 + 20 2H + 16 2D2 |
| 111 | 4,5 | 69869 | 22 2D3 + 21 2H + 15 2F1 |
| 112 | 6 | 71446 | 77 2G1 + 6 2F2 + 5 2P |
| 113 | 4,5 | 71597 | 76 2G1 + 6 2F2 + 5 2P |
| 114 | 4,5 | 72031 | 79 2G1 + 8 2F2 + 7 2P |
| 115 | 4,5 | 75303 | 44 2G1 + 13 2D1 + 13 2G2 |
| 116 | 6 | 75729 | 53 2G1 + 13 2F2 + 12 2G2 |
| 117 | 4,5 | 75826 | 52 2G1 + 13 2G2 + 11 2F2 |
| 118 | 4,5 | 78268 | 72 2G1 + 17 2S + 10 2G2 |
| 119 | 4,5 | 84683 | 89 2P + 4 2G2 + 4 2F2 |
| 120 | 4,5 | 84860 | 86 2P + 4 2F2 + 4 2G2 |
| 121 | 6 | 84892 | 87 2P + 4 2F2 + 4 2G2 |
| 122 | 6 | 95434 | 67 2D1 + 10 2D3 + 6 2H |
| 123 | 4,5 | 95438 | 67 2D1 + 10 2D3 + 6 2H |
| 124 | 6 | 96691 | 65 2D1 + 15 2D3 + 12 2G1 |
| 125 | 4,5 | 96724 | 65 2D1 + 15 2D3 + 11 2G1 |
| 126 | 4,5 | 97034 | 63 2D1 + 10 2D3 + 9 2G1 |

[a] *Labels 4,5 and 6 are abbreviations for the $\Gamma_{4,5}$ and $\Gamma_6$ irreducible representations of the $C_{3i}$ double group. Levels labeled 6 are also doublets.*

**Table 24. Energy levels ($cm^{-1}$) of $Co^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 484.80$ ($cm^{-1}$)**

| Level No. | IR[a] | Energy | Free ion state (%) |
|---|---|---|---|
| 1 | 2,3 | 0 | 100 5D |
| 2 | 1 | 8 | 100 5D |
| 3 | 1 | 165 | 100 5D |
| 4 | 2,3 | 250 | 100 5D |
| 5 | 2,3 | 373 | 99 5D |
| 6 | 1 | 512 | 97 5D + 1 1I |
| 7 | 1 | 528 | 99 5D |
| 8 | 1 | 1023 | 87 5D + 4 1I + 3 1G1 |
| 9 | 2,3 | 1057 | 99 5D |
| 10 | 2,3 | 1061 | 99 5D |
| 11 | 1 | 128 | 31 1I + 26 1G1 + 19 1G2 |
| 12 | 2,3 | 6378 | 44 3H + 23 3F2 + 16 3P1 |
| 13 | 2,3 | 6465 | 44 3H + 23 3F2 + 16 3P1 |
| 14 | 1 | 6537 | 45 3H + 23 3F2 + 16 3P1 |
| 15 | 1 | 6825 | 44 3H + 25 3F2 + 15 3P1 |
| 16 | 2,3 | 6940 | 46 3H + 24 3F2 + 14 3P1 |
| 17 | 1 | 7272 | 44 3H + 24 3F2 + 14 3P1 |
| 18 | 1 | 11037 | 34 3H + 33 3G + 16 3F1 |
| 19 | 2,3 | 11108 | 34 3H + 34 3G + 16 3F1 |
| 20 | 2,3 | 11349 | 39 3G + 29 3H + 16 3F1 |
| 21 | 2,3 | 11622 | 36 3G + 32 3H + 16 3F1 |
| 22 | 1 | 11741 | 36 3G + 32 3H + 16 3F1 |
| 23 | 1 | 11808 | 34 3H + 33 3G + 16 3F1 |
| 24 | 2,3 | 15231 | 57 1I + 22 1G1 + 18 1G2 |
| 25 | 1 | 15438 | 53 1I + 23 1G1 + 20 1G2 |
| 26 | 1 | 16256 | 99 5D |

**Table 24. Energy levels ($cm^{-1}$) of $Co^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 484.80$ ($cm^{-1}$) (cont'd)**

| Level No. | IR[a] | Energy | Free ion state (%) |
|---|---|---|---|
| 27 | 1 | 16261 | 99 5D |
| 28 | 2,3 | 16273 | 99 5D |
| 29 | 2,3 | 16289 | 99 5D |
| 30 | 1 | 16296 | 99 5D |
| 31 | 1 | 16316 | 99 5D |
| 32 | 2,3 | 16317 | 99 5D |
| 33 | 1 | 20401 | 66 3H + 27 3F2 + 5 3F1 |
| 34 | 2,3 | 20404 | 65 3H + 26 3F2 + 5 3F1 |
| 35 | 2,3 | 20643 | 65 3H + 25 3F2 + 6 3F1 |
| 36 | 2,3 | 20749 | 65 3H + 25 3F2 + 6 3F1 |
| 37 | 1 | 20828 | 67 3H + 25 3F2 + 6 3F1 |
| 38 | 1 | 20854 | 66 3H + 25 3F2 + 6 3F1 |
| 39 | 1 | 21777 | 48 3G + 47 3H + 4 3F2 |
| 40 | 1 | 21795 | 48 3G + 48 3H + 3 3F2 |
| 41 | 2,3 | 21832 | 51 3H + 44 3G + 4 3F2 |
| 42 | 2,3 | 21898 | 53 3H + 41 3G + 5 3F2 |
| 43 | 2,3 | 22466 | 54 3G + 43 3H + 2 3F2 |
| 44 | 1 | 22469 | 54 3G + 43 3H + 1 3F2 |
| 45 | 1 | 23628 | 26 1I + 21 3G + 16 3H |
| 46 | 1 | 23832 | 45 3G + 30 3P2 + 13 3H |
| 47 | 2,3 | 23863 | 44 3G + 33 3P2 + 11 3H |
| 48 | 2,3 | 23877 | 40 3G + 27 3H + 12 3D |
| 49 | 1 | 24045 | 49 3G + 32 3H + 13 3D |
| 50 | 2,3 | 24059 | 48 3G + 28 3H + 12 3D |
| 51 | 2,3 | 24265 | 46 3G + 22 3P2 + 18 3H |
| 52 | 1 | 24362 | 40 3G + 21 3P2 + 10 1I |
| 53 | 2,3 | 24365 | 46 3G + 30 3P2 + 9 3H |
| 54 | 1 | 24504 | 49 3G + 27 3P2 + 12 3H |
| 55 | 1 | 24626 | 37 3G + 15 3H + 14 3P2 |
| 56 | 2,3 | 24957 | 37 1I + 14 1D2 + 11 1F |
| 57 | 2,3 | 27783 | 49 3D + 47 3F2 + 1 3G |
| 58 | 2,3 | 27830 | 49 3D + 47 3F2 + 1 3G |
| 59 | 1 | 27868 | 49 3D + 47 3F2 + 2 3G |
| 60 | 1 | 27878 | 47 3D + 47 3F2 + 2 1I |
| 61 | 2,3 | 28094 | 53 3D + 43 3F2 + 2 1I |
| 62 | 1 | 28104 | 55 3D + 44 3F2 + 1 3F1 |
| 63 | 2,3 | 30678 | 46 1G2 + 24 1G1 + 23 1I |
| 64 | 2,3 | 30883 | 48 1I + 17 1G2 + 16 1D2 |
| 65 | 1 | 31302 | 48 1I + 15 1D2 + 12 1G2 |
| 66 | 1 | 31751 | 50 1I + 18 1S2 + 13 1G2 |
| 67 | 2,3 | 32911 | 50 3F2 + 46 3F1 + 2 1I |
| 68 | 1 | 32942 | 48 3F2 + 44 3F1 + 4 1I |
| 69 | 1 | 35653 | 27 1G2 + 24 1I + 17 3H |
| 70 | 2,3 | 35706 | 31 1G2 + 20 1I + 16 3H |
| 71 | 2,3 | 36321 | 55 3H + 18 3G + 13 3F2 |
| 72 | 1 | 36445 | 58 3H + 15 3G + 14 3F2 |
| 73 | 2,3 | 36471 | 51 3H + 17 3G + 12 3F2 |
| 74 | 1 | 36563 | 52 3H + 16 3G + 9 3F2 |
| 75 | 2,3 | 36813 | 60 3H + 27 3G + 7 3F2 |
| 76 | 1 | 36823 | 57 3H + 21 3G + 13 3F2 |
| 77 | 2,3 | 36872 | 59 3H + 32 3G + 2 3D |
| 78 | 1 | 36961 | 58 3H + 31 3G + 6 3F2 |
| 79 | 1 | 37021 | 52 1I + 33 1F + 7 3H |
| 80 | 1 | 37050 | 46 3H + 23 3G + 8 1I |
| 81 | 2,3 | 37098 | 47 3H + 20 3G + 8 3F2 |
| 82 | 2,3 | 38359 | 15 3D + 14 1F + 14 3F2 |
| 83 | 1 | 38614 | 26 3D + 25 3F2 + 19 3H |
| 84 | 1 | 38801 | 17 1F + 17 3D + 13 1G2 |
| 85 | 2,3 | 38868 | 16 1F + 14 3F2 + 14 1I |
| 86 | 1 | 39292 | 30 3D + 26 3F2 + 18 3H |
| 87 | 2,3 | 39475 | 30 3D + 26 3F2 + 18 3H |
| 88 | 1 | 39564 | 19 1F + 15 3D + 13 3F2 |
| 89 | 2,3 | 39653 | 31 3D + 26 3F2 + 18 3H |
| 90 | 2,3 | 39784 | 97 3G + 1 3F2 + 1 3H |
| 91 | 1 | 39787 | 96 3G + 1 3F2 + 1 3H |
| 92 | 2,3 | 41737 | 29 3P2 + 26 3G + 23 3F2 |
| 93 | 2,3 | 41828 | 31 3P2 + 25 3G + 23 3F2 |
| 94 | 1 | 41919 | 32 3P2 + 25 3G + 22 3F2 |
| 95 | 1 | 41952 | 34 3P2 + 25 3G + 22 3F2 |
| 96 | 2,3 | 42600 | 33 3P2 + 28 3G + 20 3F2 |
| 97 | 1 | 42613 | 34 3P2 + 28 3G + 20 3F2 |
| 98 | 2,3 | 43976 | 33 1D2 + 23 1I + 23 1G1 |
| 99 | 1 | 44046 | 80 3D + 15 3G + 2 1I |
| 100 | 1 | 44061 | 82 3D + 15 3G + 2 3H |
| 101 | 2,3 | 44067 | 81 3D + 15 3G + 2 3H |
| 102 | 2,3 | 44097 | 82 3D + 15 3G + 2 3H |
| 103 | 1 | 45367 | 50 1I + 19 1D2 + 19 1G1 |
| 104 | 2,3 | 45741 | 46 1I + 24 1D2 + 19 1G1 |
| 105 | 2,3 | 49708 | 41 1I + 31 1G2 + 18 1D2 |
| 106 | 1 | 49839 | 60 1F + 38 1I + 1 1G1 |
| 107 | 1 | 50546 | 40 1S2 + 40 1G2 + 11 1S1 |
| 108 | 2,3 | 52683 | 72 1F + 10 1I + 10 1G1 |
| 109 | 1 | 53530 | 76 1F + 9 1I + 7 1G1 |
| 110 | 1 | 54027 | 51 3F1 + 47 3F2 + 1 3P1 |
| 111 | 2,3 | 54032 | 51 3F1 + 47 3F2 + 1 3P1 |
| 112 | 1 | 55108 | 46 1G2 + 33 1F + 11 1G1 |
| 113 | 2,3 | 55641 | 48 1G2 + 34 1F + 8 1G1 |
| 114 | 1 | 57473 | 58 3P1 + 12 3F1 + 9 3H |

**Table 24. Energy levels ($cm^{-1}$) of $Co^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 484.80$ ($cm^{-1}$) (cont'd)**

| Level No. | IR[a] | Energy | Free ion state (%) | Level No. | IR[a] | Energy | Free ion state (%) |
|---|---|---|---|---|---|---|---|
| 115 | 1 | 57542 | 56 3P1 + 14 3F1 + 9 3H | 129 | 1 | 64043 | 61 3F1 + 11 3P2 + 7 3F2 |
| 116 | 2,3 | 57570 | 55 3P1 + 15 3F1 + 9 3H | 130 | 2,3 | 65366 | 58 3F1 + 15 3P2 + 8 3P1 |
| 117 | 2,3 | 57791 | 48 3P1 + 23 3F1 + 9 3H | 131 | 1 | 65388 | 60 3F1 + 13 3P2 + 8 3G |
| 118 | 2,3 | 58032 | 57 3P1 + 15 3F1 + 10 3H | 132 | 2,3 | 65395 | 57 3F1 + 15 3P2 + 9 3P1 |
| 119 | 1 | 58061 | 57 3P1 + 14 3F1 + 10 3H | 133 | 1 | 65399 | 60 3F1 + 14 3P2 + 8 3G |
| 120 | 2,3 | 59977 | 63 3F1 + 15 3F2 + 7 3D | 134 | 1 | 69443 | 62 1G1 + 33 1G2 + 3 1I |
| 121 | 2,3 | 60007 | 64 3F1 + 15 3F2 + 8 3D | 135 | 2,3 | 69469 | 59 1G1 + 32 1G2 + 4 1F |
| 122 | 1 | 60048 | 66 3F1 + 16 3F2 + 9 3D | 136 | 1 | 70869 | 53 1G1 + 22 1G2 + 14 1S2 |
| 123 | 1 | 60099 | 64 3F1 + 15 3F2 + 9 3D | 137 | 2,3 | 73112 | 41 1D2 + 34 1G1 + 17 1G2 |
| 124 | 2,3 | 60776 | 68 3F1 + 19 3F2 + 9 3D | 138 | 2,3 | 76771 | 78 1D1 + 10 1G1 + 6 1I |
| 125 | 1 | 60806 | 68 3F1 + 19 3F2 + 9 3D | 139 | 2,3 | 87513 | 73 1D1 + 15 1D2 + 9 1F |
| 126 | 2,3 | 61798 | 66 1G1 + 20 1I + 9 1D2 | 140 | 1 | 88855 | 71 1D1 + 16 1D2 + 9 1F |
| 127 | 1 | 62077 | 62 1G1 + 19 1I + 10 1D2 | 141 | 1 | 108376 | 71 1S1 + 13 1S2 + 11 1G1 |
| 128 | 2,3 | 63996 | 63 3F1 + 11 3P2 + 7 3F2 | | | | |

[a]*Labels 1 and 2,3 are abbreviations for the $\Gamma_1$ and $\Gamma_{2,3}$ irreducible representations of the $C_{3i}$ group.*

**Table 25. Energy levels ($cm^{-1}$) of $Ni^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 599.20$ ($cm^{-1}$)**

| Level No. | IR[a] | Energy | Free ion state (%) | Level No. | IR[a] | Energy | Free ion state (%) |
|---|---|---|---|---|---|---|---|
| 1 | 4,5 | 0 | 94 4F + 6 4P | 22 | 4,5 | 22407 | 61 2P + 21 2H + 13 2F |
| 2 | 6 | 354 | 92 4F + 7 4P | 23 | 4,5 | 22948 | 62 2P + 22 2H + 13 2F |
| 3 | 4,5 | 385 | 94 4F + 5 4P | 24 | 4,5 | 25548 | 87 4P + 12 4F + 1 2P |
| 4 | 4,5 | 908 | 90 4F + 6 4P + 2 2G | 25 | 6 | 25648 | 85 4P + 12 4F + 1 2P |
| 5 | 6 | 910 | 91 4F + 6 4P + 2 2G | 26 | 4,5 | 26478 | 94 4P + 6 4F |
| 6 | 4,5 | 1109 | 94 4F + 6 4P | 27 | 6 | 26799 | 91 4P + 6 4F + 1 2H |
| 7 | 4,5 | 4682 | 42 2G + 28 2H + 13 2D2 | 28 | 4,5 | 26989 | 92 4P + 5 4F + 1 2H |
| 8 | 6 | 4729 | 43 2G + 29 2H + 13 2D2 | 29 | 4,5 | 27143 | 91 4P + 5 4F + 1 2P |
| 9 | 6 | 14038 | 97 4F + 2 2G + 1 2D2 | 30 | 4,5 | 29650 | 88 4F + 5 4P + 3 2H |
| 10 | 4,5 | 14066 | 98 4F + 1 2G | 31 | 6 | 29656 | 87 4F + 5 4P + 4 2H |
| 11 | 4,5 | 14305 | 98 4F + 1 2G | 32 | 4,5 | 30250 | 97 2G + 1 2H + 1 2P |
| 12 | 6 | 14350 | 97 4F + 2 2G | 33 | 4,5 | 31055 | 55 2H + 28 2G + 9 2D1 |
| 13 | 4,5 | 14383 | 95 4F + 3 2G + 1 2D2 | 34 | 6 | 31307 | 54 2H + 24 2G + 9 2D1 |
| 14 | 4,5 | 14624 | 98 4F + 1 2G | 35 | 4,5 | 31594 | 59 2H + 22 2G + 8 2D1 |
| 15 | 4,5 | 17383 | 50 2G + 46 2H + 2 4F | 36 | 6 | 33728 | 66 2H + 19 2G + 12 2P |
| 16 | 6 | 17542 | 53 2G + 42 2H + 2 4F | 37 | 4,5 | 33838 | 66 2H + 21 2G + 11 2P |
| 17 | 4,5 | 17995 | 51 2G + 46 2H + 2 4F | 38 | 4,5 | 33937 | 61 2H + 27 2G + 10 2P |
| 18 | 4,5 | 18248 | 59 2G + 16 2H + 15 2D2 | 39 | 4,5 | 35857 | 53 2H + 37 2D2 + 8 2D1 |
| 19 | 6 | 18272 | 58 2G + 16 2H + 16 2D2 | 40 | 6 | 35909 | 52 2H + 37 2D2 + 9 2D1 |
| 20 | 4,5 | 18424 | 57 2G + 19 2D2 + 15 2H | 41 | 4,5 | 38962 | 72 2D2 + 12 2G + 11 2H |
| 21 | 6 | 22265 | 60 2P + 21 2H + 12 2F | 42 | 4,5 | 39156 | 68 2D2 + 17 2H + 11 2G |

**Table 25. Energy levels ($cm^{-1}$) of $Ni^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 599.20$ ($cm^{-1}$) (cont'd)**

| Level No. | IR[a] | Energy | Free ion state (%) | Level No. | IR[a] | Energy | Free ion state (%) |
|---|---|---|---|---|---|---|---|
| 43 | 6 | 39210 | 69 2D2 + 18 2H + 10 2G | 52 | 4,5 | 48499 | 100 2F |
| 44 | 4,5 | 40856 | 48 2H + 38 2F + 13 2G | 53 | 6 | 51917 | 43 2F + 24 2P + 18 2H |
| 45 | 4,5 | 41769 | 45 2F + 40 2H + 9 2G | 54 | 4,5 | 52066 | 44 2F + 24 2P + 18 2H |
| 46 | 6 | 41894 | 45 2F + 40 2H + 11 2G | 55 | 4,5 | 52796 | 48 2F + 25 2P + 16 2H |
| 47 | 4,5 | 42731 | 73 2F + 15 2H + 8 2D1 | 56 | 4,5 | 68497 | 65 2D1 + 31 2D2 + 3 2H |
| 48 | 6 | 43482 | 77 2F + 11 2H + 8 2D1 | 57 | 6 | 68511 | 64 2D1 + 32 2D2 + 3 2H |
| 49 | 4,5 | 43799 | 78 2F + 10 2D1 + 9 2H | 58 | 4,5 | 71390 | 76 2D1 + 12 2F + 6 2H |
| 50 | 6 | 46346 | 53 2G + 17 2H + 15 2D1 | 59 | 6 | 72396 | 75 2D1 + 12 2F + 7 2D2 |
| 51 | 4,5 | 46352 | 53 2G + 16 2H + 15 2D1 | 60 | 4,5 | 72890 | 73 2D1 + 13 2F + 8 2D2 |

[a]*Labels 4,5 and 6 are abbreviations for the $\Gamma_{4,5}$ and $\Gamma_6$ irreducible representations of the $C_{3i}$ double group. Levels labeled 6 are also doublets.*

**Table 26. Energy levels ($cm^{-1}$) of $Cu^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 728.80$ ($cm^{-1}$)**

| Level No. | IR[a] | Energy | Free ion state (%) | Level No. | IR[a] | Energy | Free ion state (%) |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 0 | 100 3F | 16 | 1 | 26964 | 85 1G + 10 1S + 3 3F |
| 2 | 2,3 | 3 | 100 3F | 17 | 2,3 | 29617 | 74 1D + 21 1G + 3 3P |
| 3 | 2,3 | 1400 | 281 3F + 13 1D + 6 1G | 18 | 1 | 303[illegible] | 71 1D + 25 1G + 3 3P |
| 4 | 2,3 | 14434 | 99 3F | 19 | 2,3 | 34653 | 80 1G + 15 3P + 5 3F |
| 5 | 1 | 14583 | 100 3F | 20 | 1 | 34780 | 44 1G + 42 3P + 14 3F |
| 6 | 1 | 14814 | 100 3F | 21 | 2,3 | 35026 | 57 3P + 29 3F + 13 1G |
| 7 | 2,3 | 15000 | 98 3F + 1 1D + 1 1G | 22 | 1 | 35114 | 70 3P + 27 3F + 1 1D |
| 8 | 1 | 15162 | 100 3F | 23 | 2,3 | 35133 | 61 3P + 30 3F + 7 1G |
| 9 | 2,3 | 15969 | 53 1D + 24 1G + 22 3F | 24 | 1 | 35388 | 56 1G + 30 3P + 14 3F |
| 10 | 1 | 21784 | 74 3F + 24 3P + 2 1G | 25 | 2,3 | 36821 | 71 3P + 27 3F + 1 1G |
| 11 | 2,3 | 22141 | 74 3F + 26 3P | 26 | 1 | 36855 | 71 3P + 27 3F + 1 1G |
| 12 | 1 | 22698 | 72 3F + 27 3P | 27 | 1 | 46631 | 75 1G + 25 1D |
| 13 | 1 | 22893 | 68 3F + 31 3P | 28 | 2,3 | 46686 | 68 1G + 32 1D |
| 14 | 2,3 | 23128 | 67 3F + 32 3P | 29 | 2,3 | 47877 | 77 1G + 23 1D |
| 15 | 2,3 | 23313 | 65 3F + 33 3P + 1 1G | 30 | 1 | 72868 | 89 1S + 11 1G |

[a]*Labels 1 and 2,3 are abbreviations for the $\Gamma_1$ and $\Gamma_{2,3}$ irreducible representations of the $C_{3i}$ group.*

**Table 27. Energy levels ($cm^{-1}$) of $Zn^{3+}$ in $Y_3Al_5O_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 923.88^a$ ($cm^{-1}$)**

| Level No. | IR[b] | Energy | Free ion state (%) |
|---|---|---|---|
| 1 | 6 | 0 | 100 2D |
| 2 | 4,5 | 105 | 100 2D |
| 3 | 4,5 | 13303 | 100 2D |
| 4 | 4,5 | 14616 | 100 2D |
| 5 | 6 | 15116 | 100 2D |

*[a]Hartree-Fock value (ref 18).*
*[b]Labels 4,5 and 6 are abbreviations for the $\Gamma_{4,5}$ and $\Gamma_6$ irreducible representations of the $C_{3i}$ double group. Levels labeled 6 are also doublets.*

## 4.2 Discussion of Results

Because of the sparse experimental data on the fine structure, a detailed comparison of the calculation given in tables 19 through 27 is not possible. The only ion with reliable fine structure reported is $Cr^{3+}$ [7, 9, 10, 22], and these data were used to determine the crystal field parameter $B_{20}$ for $Cr^{3+}$.

The results given for $Ti^{3+}$ in table 19 show considerable splitting of the lower levels, but since only room temperature absorption was reported by Karpov et al [4], no comparison can be made. The absorption spectra at room temperature were reported by Bantien et al [23] as having bands at 25,600, 19,800, and 17,100 $cm^{-1}$, with the band at 25,600 $cm^{-1}$ being very strong compared to the other two bands. The two lower energy bands were assumed to be $3d^1 \rightarrow 3d^1$ transitions, but the high-energy band is unknown and under investigation.

The energy levels of $V^{3+}$ given in table 20 show considerable splitting of the ground state ($^3T_1$ in cubic approximation) so that if the absorption spectra were taken at low temperature rather than at room temperature as reported by Weber and Riseberg [5], the lines should be much narrower. Surprisingly, the spin-orbit and the two-fold field $B_{20}$ do not mix the states much, and the usual assumption of spin-forbidden transitions in the analysis of the absorption spectra should be reasonably valid. It should be interesting to analyze the spectra taken at low temperature.

There are a considerable number of papers reporting the experimental data and analysis of experimental data on $Cr^{3+}$ in YAG. The calculated splitting of the ground state, 0.62 $cm^{-1}$, is slightly larger than the experimental value [10] 0.53 $cm^{-1}$, but the splitting of the $R$ lines calculated to be 19.5 $cm^{-1}$ compares well with the experimental value [10] 19.6 $cm^{-1}$ (levels 3 and 4 in table 21). The calculated centroid of the $R$ lines is shifted approximately 600 $cm^{-1}$ from the experimental value reported by Henry et al [10]. Comparison of the results in table 21 with the experimental results given in tables 4 through 7 shows, in general, that the calculated values are slightly higher than the experimental results. Slight adjustment of the parameters can bring the calculated values into better agreement with any one set of the experimental results. Also, mixing of the states by the spin-orbit does not occur below level number 32 (37,935 $cm^{-1}$) in table 21, which should make identification of the fine structure somewhat easier.

Using the parameters of table 17, we calculated the energy levels for $Mn^{3+}$, and the results are given in table 22. For this set of parameters, the high spin state $^5D$ is the lowest, which contradicts the assumptions made by Arsenov and Sviridov [11] in analyzing the experimental data. However, only three energy levels were reported so that a re-analysis of the experimental data would be inconclusive. We found that if we reduced $F^{(4)}$ from 41,688 $cm^{-1}$ to 33,332 $cm^{-1}$, the ground state became mixed with the $^3H$ levels (the low spin ground states assumed in ref 11).

The energy levels of $Fe^{3+}$ given in table 23 were obtained using the parameters given in table 17 with $\alpha$ = 30 $cm^{-1}$ and $\gamma$ = 0. The ground state ($^6A_1$ in the cubic approximation) is split by the spin orbit and the two-fold field, $B_{20}$. We have been unable to find any reported measurement of this ground state splitting. The spin-orbit coupling mixes the spin of a large number of levels, and the calculated energy levels appear to be considerably higher than experiment. We have not tried to fit the experimental data starting with the parameters of table 23. A comparison of the parameters obtained here for $Fe^{3+}$ in YAG with the parameters for $Fe^{3+}$ in $Ho_3Al_5O_{12}$ or $Er_3Al_5O_{12}$ shows that the $F^{(k)}$ for YAG are larger but $B_{20}$ is smaller than these compounds [2]. The $B_{40}$ and $B_{43}$ crystal field parameters are approximately the same. The experimental data for $Fe^{3+}$ in the rare earth garnets were considerably different than reported for $Fe^{3+}$ in YAG [12,13].

The energy levels for $Co^{3+}$ were calculated using the parameters given in table 17 with $\alpha = 30\ cm^{-1}$ and $\gamma = 0$; the results are given in table 24. As for $Mn^{3+}$, the calculated ground state disagrees with that given by Arsenev and Sviridov [11]. However, we have observed that a reduction of the parameter $\alpha$ causes the ground state, which in table 24 is predominately $^5D$, to become significantly mixed with $^3F_2$, $^3H$, and $^1I$. If more data were available, a fitting starting with the parameters of table 17 could be undertaken.

The energy levels for $Ni^{3+}$, $Cu^{3+}$, and $Zn^{3+}$ were calculated using the parameters in table 17. We are unaware of any data reported on these ions in YAG, and we are uncertain as to the possibility of doping YAG with these ions. It would seem that doping with $Ni^{3+}$ would be possible since the spectrum of this ion in the rare earth garnets has been reported [24].

**Author's note**: Since this report has been written an article has appeared (in Russian) by Yu. A. Voitukevich, M. V. Konzhik, V. V. Kuz'min, M. G. Livshitz and M. L. Meil'man: *Energy Structure of $Fe^{3+}$ Impurity Ions in Yttrium Aluminum Garnet ($Y_3Al_5O_{12}$) Crystals*, Opt. Spectrosc. *63* (1987), 810. Consequently, a supplement to this report will be issued which will include an analysis of this latest data.

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